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A Study of Industrial Data on Candidate Chemicals for Testing

SRI International, Menlo Park, Calif

Prepared for

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A STUDY OF INDUSTRIAL DATA ON CANDIDATE CHEMICALS FOR TESTING

August 1977

Research Request No. 1

FINAL REPORT

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16. ABSTRACT

This report summarizes the work done under Research Request No. 1 and includes three major parts:

(1) Data previously collected on an NSF study was supplemented to provide the following information where available on 667 industrial chemicals: (a) U.S. production; (b) estimates of quantities released annually to the environment; (c) major uses; and (d) references on mutagenicity tests. Mutagenicity data on 25 chemicals were evaluated after developing a list of assays and criteria for classifying the results as either positive or negative/inadequate.

(2) Tables were prepared which contain economic information on 1791 chemicals belonging to 26 structural classes considered to represent potential industrial carcinogens and mutagens. For those chemicals with annual production greater than one million pounds, market forecasts were prepared which present a brief summary of production, consumption patterns, major uses, possible substitutes, and growth trends.

(3) Carcinogenicity data for all chemicals belonging to three classes (epoxides, alkyl halides, and vinyl halides) were used to correlate structural features with carcinogenic activity. Criteria were developed for estimating the potential carcinogenicity of chemicals in each class. These criteria were applied to those chemicals in each class known to be produced commercially or for which there was evidence of significant human exposure. The results of the study were summarized in three separate reports.

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Mutagens	Environmental Release	06/05	05/03
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A STUDY OF INDUSTRIAL DATA ON CANDIDATE CHEMICALS FOR TESTING

August 1977

Contract No. 68-01-4109
Research Request No. 1

Project Officer: James Darr

Prepared for

Office of Toxic Substances
U.S. Environmental Protection Agency
Washington, D.C. 20460

NOTICE

This report has been reviewed by the Office of Toxic Substances, EPA, and approved for publication. Approval does not signify that the contents necessarily reflect the views and policies of the Environmental Protection Agency, nor does mention of trade names or commercial products constitute endorsement or recommendation for use.

PREFACE

This report was prepared by an interdisciplinary team under the general guidance of the two EPA project officers, Rosalind Schoof and James Darr. The SRI team consisted of Jeffrey Allport, Sharon Casey, Janet Cook, Peter Hall, C. Tucker Helmes, Oscar Johnson, Barbara Lewin, Kirtland McCaleb (Project Leader), Ann Mitchell, Gordon Newell, Meg Power, Shirley Radding, Caroline Sigman, Vincent Simmon, Cecilia Smith, Susanne Urso, Anita Van Der Tak, Janet Walker, and Rose Wright.

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ATTENTION

AS NOTED IN THE NTIS ANNOUNCEMENT, PORTIONS OF THIS REPORT ARE NOT LEGIBLE. HOWEVER, IT IS THE BEST REPRODUCTION AVAILABLE FROM THE COPY SENT TO NTIS.

I. INTRODUCTION

A. Background

The Office of Toxic Substances of the Environmental Protection Agency needs to produce information packages as a basis for decisions about testing chemicals for unreasonable risk to human health or the environment. Contract No. 68-01-4109 with SRI International (formerly Stanford Research Institute) was established as a first step in producing these packages. It calls for SRI to provide, in answer to Research Requests provided by the Project Officer, selected economic, chemical, and biological information on selected commercial chemicals.

B. Objectives

The objectives of the study reported in this document were as follows:

- Utilize economic and toxicologic information developed in previous projects for the National Science Foundation (NSF) and the National Cancer Institute (NCI) to provide data on commercially significant chemicals. (The NSF project provided information on the 250 chemicals with the greatest potential for environmental effects based on their estimated release to the environment during their production and use. Information developed as part of an NCI project and used specifically for this contract consisted of Stage I and Stage II dossiers, which provide exposure and use information as well as indicators of potential carcinogenicity and physical, chemical, and biological properties for specific chemicals.)

- Identify those chemicals whose mutagenic properties have been studied and provide an evaluation of the test results on 25 chemicals selected by the Project Officer.
- Expand a list of 72 chemicals identified by EPA as potential industrial carcinogens and mutagens in order to include all the chemicals in the ten major classes represented by the 72 chemicals.
- Identify the commercially significant chemicals belonging to each of the ten major classes (and their numerous structural classes), subdivide them according to annual production volume, and prepare tables of economic data for the chemicals with annual production of (a) one million pounds or more, and (b) one thousand pounds or more.
- Prepare market forecasts for the chemicals with annual production of one million pounds or more.
- Prepare reports on the results of studies of the potential carcinogenicity of the members of the epoxide, alkyl halide, and vinyl halide classes based on structure-activity analysis.

II. SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

A. Summary

This report describes the work carried out on Research Request No. 1 as specified by the Project Officer during the course of the study.

In one of the two major parts of the study, data previously collected on 667 organic chemicals as part of a project for the National Science Foundation (NSF) were reorganized and supplemented with additional data to provide the following information on the chemicals where available: (a) data on U.S. annual production; (b) estimates of the quantities released annually to the environment; (c) identification of major uses; and (d) accession numbers for any references on mutagenicity tests that are available in the files of the Environmental Mutagen Information Center (EMIC). The mutagenicity data on 25 chemicals selected by the Project Officer were then evaluated after developing a list of assays and criteria for classifying the results as either positive or negative/inadequate.

In the second major part of the study, a list of 72 chemicals considered to represent potential industrial carcinogens and mutagens was expanded to a total of 1791 chemicals by a review of sources which identify commercial chemicals. Data relating to the commercial importance of these chemicals were gathered and compiled into tables for each of 26 structural classes. For those chemicals in each of these structural classes which could be identified as having an annual U.S. production equal to or greater than one million pounds (a total of 109 chemicals), so-called "market forecasts" were prepared which present a brief summary of production and trade statistics, consumption patterns and descriptions of major and potential uses, identification of possible substitutes, and growth trends.

An additional task assigned by the Project Officer was a study of the potential carcinogenicity of selected chemicals based on structure-activity analysis. A review was made of the carcinogenicity data for all chemicals belonging to the three classes (epoxides, alkyl halides, and vinyl halides) selected by the Project Officer. This was used to correlate structural features with carcinogenic activity and criteria were developed for estimating the potential carcinogenicity of chemicals in each class. These criteria were applied to the chemicals in the class known to be produced commercially or for which there was evidence of significant human exposure. The results of the study of the classes were summarized in three separate reports.

B. Conclusions and Recommendations

Because Research Request No. 1 was designed to provide certain specified information on selected chemicals, no conclusions were drawn from the studies performed.

If the Office of Toxic Substances finds the information provided in this report to be useful, we recommend the following additional studies to supplement those described in this report:

- Evaluation of the mutagenicity data on additional chemicals from the NSF study, and on other chemicals identified as having significant human exposure.
- Preparation of economic data tables and market forecasts on the chemicals in any additional classes (anthraquinones, aromatic hydrocarbons, cyclic ethers, heterocyclic amines, phosphoramides, etc.) studied by Dr. Fishbein.
- Evaluation of the potential carcinogenicity of the chemicals in additional classes based on structure-activity analysis.

III. STUDY OF CHEMICALS FROM A NATIONAL SCIENCE FOUNDATION STUDY

A. Preparation of Tables Containing Economic Information

In this part of Research Request No. 1, SRI produced computer-generated tables containing economic information on commercially significant chemicals. These chemicals had previously been identified as having an annual production volume greater than one million pounds in 1972, 1971, or 1970 in an earlier SRI project done for the National Science Foundation (NSF).

For the present study, Chemical Abstracts Services Registry numbers (CAS numbers) were obtained for as many of these NSF chemicals as possible. The chemicals were then divided into those with CAS numbers (436 chemicals) and those without CAS numbers (231 chemicals, groups, or mixtures). Tables 3-1 and 3-2 contain these chemicals listed in order of decreasing annual production, along with additional information: (1) the production quantity, data source, and year; (2) the use category of the chemical as designated by the U.S. International Trade Commission (e.g., dyes, pesticides, plasticizers); and (3) the estimated annual release potential (a rough estimate of potential annual losses to the environment which was available for approximately one-third of the chemicals from the NSF study).

Some of the columns in Tables 3-1 and 3-2 need some additional explanation:

1. Production

A production level of one million pounds was chosen as the one above which a chemical was considered to be an important commodity chemical. Due to the common usage of one million pounds production as a measure of a commodity chemical, and in keeping with the units used by the International Trade Commission in its series, Synthetic Organic Chemicals, U.S. Production and Sales, the use of the pound as a unit of weight has been adopted for all of the sections of this report dealing with economic aspects of the chemicals.

2. Source

The production figures are either reported data from Synthetic Organic Chemicals, U.S. Production and Sales, published by the U.S. International Trade Commission and designated as T72 (for 1972), T71 (for 1971), or T70 (for 1970), or are SRI estimates, designated as SRI.

3. Use Category

This is one of the following 14 major groupings used in Synthetic Organic Chemicals:

Category	Abbreviation Used
Tar and tar crudes	Tar & tar crudes
Crude products from petroleum and natural gas for chemical conversion	Crude products
Cyclic intermediates	Cyclic intermed
Dyes	Dyes
Organic pigments	Org pigments
Medicinal chemicals	Medicinal chems
Flavor and perfume materials	Flavor & perfume
Plastics and resin materials	Plastic & resin
Rubber-processing chemicals	Rubber-proc chem
Elastomers	Elastomers
Plasticizers	Plasticizers
Surface-active agents	Surf-activ agent

Category	Abbreviation Used
Pesticides and related products	Pesticides
Miscellaneous chemicals	Misc chems

4. Release Rate

The release rate, R, was calculated for a number of chemicals on a previous project done for NSF and is defined as follows:

$$R = C\ (F_D) + P\ (F_{PL})$$

where C is the apparent U.S. annual consumption, F_D is the fraction of the annual consumption of the chemical that goes to nonintermediate dispersive uses, P is the annual U.S. production, and F_{PL} is the fraction of the annual U.S. production that is lost and escapes from the plant site during the manufacture of the chemical.

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Table 3-1. INDUSTRIAL CHEMICALS WITH CAS NUMBERS

Total No. 436

CAS	NAME	PRODUCTION	SOURCE	USE CATEGORY	RELEASE POTENTIAL
000074851	ETHYLENE	20812.1 MIL LBS	T72	CRUDE PRODUCTS	521.3 MIL LBS
000057136	UREA	15320.0 MIL LBS	SRI	MISC CHEMS	1162.1 MIL LBS
000074986	PROPANE	9668.3 MIL LBS	T72	CRUDE PRODUCTS	96.1 MIL LBS
000071432	BENZENE	8937.1 MIL LBS	T72	CRUDE PRODUCTS	113.6 MIL LBS
000107062	1,2-DICHLOROETHANE (ETHYLENE DICHLORIDE)	8600.0 MIL LBS	SRI	MISC CHEMS	540.2 MIL LBS
000115071	PROPYLENE	8471.6 MIL LBS	T72	CRUDE PRODUCTS	127.1 MIL LBS
008032324	SOLVENT NAPHTHA	8216.4 MIL LBS	T72	TAR & TAR CRUDES	1371.3 MIL LBS
000100414	ETHYLBENZENE	6920.0 MIL LBS	SRI	CYCLIC INTERMED	203.5 MIL LBS
000067561	METHANOL, SYNTHETIC	6060.1 MIL LBS	T72	MISC CHEMS	987.7 MIL LBS
000100425	STYRENE, ALL GRADES	5940.7 MIL LBS	T72	CYCLIC INTERMED	89.1 MIL LBS
000108883	TOLUENE	5917.2 MIL LBS	T72	CRUDE PRODUCTS	1074.2 MIL LBS
000050000	FORMALDEHYDE (37% BY WEIGHT)	5651.8 MIL LBS	T72	MISC CHEMS	52.3 MIL LBS
000074840	ETHANE	5136.5 MIL LBS	T72	CRUDE PRODUCTS	11.4 MIL LBS
000075014	VINYL CHLORIDE, MONOMER (CHLOROETHYLENE)	5088.5 MIL LBS	T72	MISC CHEMS	146.5 MIL LBS
009002862	POLYVINYL CHLORIDE	4258.0 MIL LBS	SRI	PLASTIC & RESIN	4365.7 MIL LBS
000075218	ETHYLENE OXIDE	3961.8 MIL LBS	T72	MISC CHEMS	98.8 MIL LBS
000106990	1,3-BUTADIENE, GRADE FOR RUBBERS (ELASTOMERS)	3791.3 MIL LBS	SRI	CRUDE PRODUCTS	56.9 MIL LBS
000107211	ETHYLENE GLYCOL	3761.1 MIL LBS	T72	MISC CHEMS	2526.3 MIL LBS
009003558	POLYBUTADIENE-STYRENE ELASTOMERS	2510.1 MIL LBS	T72	ELASTOMERS	2556.7 MIL LBS
009003683	POLYETHYLENE TEREPHTHALATE	2506.0 MIL LBS	SRI	MISC CHEMS	2487.5 MIL LBS
000106978	N-BUTANE	2331.1 MIL LBS	T72	CRUDE PRODUCTS	23.3 MIL LBS
000110827	CYCLOHEXANE	2258.4 MIL LBS	T72	CYCLIC INTERMED	94.2 MIL LBS
000098828	CUMENE	2292.9 MIL LBS	T72	CYCLIC INTERMED	50.3 MIL LBS
000064197	ACETIC ACID, SYNTHETIC, 100%	2235.0 MIL LBS	T72	MISC CHEMS	55.9 MIL LBS
000120616	TEREPHTHALIC ACID, DIMETHYL ESTER	2147.3 MIL LBS	T72	CYCLIC INTERMED	32.5 MIL LBS
000106423	P-XYLENE	2098.2 MIL LBS	SRI	CYCLIC INTERMED	39.9 MIL LBS
000100210	TEREPHTHALIC ACID	1928.9 MIL LBS	T72	CYCLIC INTERMED	28.9 MIL LBS
000108952	PHENOL	1915.5 MIL LBS	SRI	CYCLIC INTERMED	47.0 MIL LBS
000064175	ETHYL ALCOHOL, SYNTHETIC	1850.7 MIL LBS	T72	MISC CHEMS	581.7 MIL LBS
000067630	ISOPROPYL ALCOHOL	1790.0 MIL LBS	T72	MISC CHEMS	876.2 MIL LBS
009003070	POLYPROPYLENE	1730.9 MIL LBS	T72	PLASTIC & RESIN	1583.2 MIL LBS
000067641	ACETONE	1704.1 MIL LBS	SRI	MISC CHEMS	553.9 MIL LBS
000075569	PROPYLENE OXIDE	1640.0 MIL LBS	T72	MISC CHEMS	40.8 MIL LBS
000108247	ACETIC ANHYDRIDE, 100%	1572.9 MIL LBS	T72	MISC CHEMS	39.4 MIL LBS
000124049	ADIPIC ACID	1491.4 MIL LBS	T72	MISC CHEMS	37.3 MIL LBS
000075070	ACETALDEHYDE	1447.6 MIL LBS	T72	MISC CHEMS	36.2 MIL LBS
000108054	VINYL ACETATE	1210.7 MIL LBS	T72	MISC CHEMS	18.2 MIL LBS
009003536	POLYSTYRENE, STRAIGHT	1157.3 MIL LBS	T72	PLASTIC & RESIN	1471.0 MIL LBS
000107131	ACRYLONITRILE	1114.7 MIL LBS	T72	MISC CHEMS	27.4 MIL LBS
000075650	TERT-BUTYL ALCOHOL	1000.0 MIL LBS	SRI	MISC CHEMS	715.0 MIL LBS
000056235	CARBON TETRACHLORIDE	996.7 MIL LBS	T72	MISC CHEMS	105.0 MIL LBS
000075285	ISOBUTANE	942.1 MIL LBS	T72	CRUDE PRODUCTS	
000085449	PHTHALIC ANHYDRIDE	913.0 MIL LBS	T72	CYCLIC INTERMED	14.0 MIL LBS
009003569	ACRYLONITRILE-BUTADIENE-STYRENE	863.7 MIL LBS	T72	PLASTIC & RESIN	911.6 MIL LBS
000124094	1,6-HEXANEDIAMINE (HEXAMETHYLENEDIAMINE)	856.4 MIL LBS	T72	MISC CHEMS	12.8 MIL LBS
000095476	O-XYLENE	831.8 MIL LBS	T72	CYCLIC INTERMED	
009004357	CELLULOSE ACETATE	807.1 MIL LBS	T72	MISC CHEMS	24.6 MIL LBS
000108941	CYCLOHEXANONE	784.4 MIL LBS	T72	CYCLIC INTERMED	51.0 MIL LBS
000075150	CARBON DISULFIDE	767.6 MIL LBS	T72	MISC CHEMS	49.9 MIL LBS
000127184	TETRACHLOROETHYLENE (PERCHLOROETHYLENE)	734.2 MIL LBS	T72	MISC CHEMS	588.0 MIL LBS
009003172	STEREO POLYBUTADIENE	666.4 MIL LBS	T72	ELASTOMERS	729.5 MIL LBS
000105602	CAPROLACTAM	640.0 MIL LBS	T72	MISC CHEMS	

Table 3-1 (continued)

000075445	PHOSGENE (CARBONYL CHLORIDE)	637.0 MIL LBS	T72	MISC CHEMS	
000115117	ISOBUTYLENE	600.2 MIL LBS	T72	CRUDE PRODUCTS	
000080626	METHYL METHACRYLATE	599.0 MIL LBS	T72	MISC CHEMS	
000071363	N-BUTYL ALCOHOL	590.2 MIL LBS	T72	MISC CHEMS	144.6 MIL LBS
000075003	ETHYL CHLORIDE (CHLOROETHANE)	575.5 MIL LBS	T72	MISC CHEMS	34.5 MIL LBS
000057556	PROPYLENE GLYCOL	562.6 MIL LBS	T72	MISC CHEMS	154.6 MIL LBS
000098953	NITROBENZENE	551.2 MIL LBS	T72	CYCLIC INTERMED	19.3 MIL LBS
009003558	STYRENE-BUTADIENE COPOLYMER	549.0 MIL LBS	T72	PLASTIC & RESIN	510.5 MIL LBS
000091178	NAPHTHALENE	535.2 MIL LBS	SRI	CRUDE PRODUCTS	16.9 MIL LBS
000104767	2-ETHYL-1-HEXANOL	526.1 MIL LBS	T72	MISC CHEMS	70.0 MIL LBS
000078933	2-BUTANONE (METHYL ETHYL KETONE)	509.0 MIL LBS	T72	MISC CHEMS	524.7 MIL LBS
000075092	DICHLOROMETHANE (METHYLENE CHLORIDE)	471.3 MIL LBS	T72	MISC CHEMS	366.8 MIL LBS
008052480	TALLOW ACIDS, SODIUM SALT	465.6 MIL LBS	T72	SURF-ACTIV AGENT	479.5 MIL LBS
000074873	CHLOROMETHANE (METHYL CHLORIDE)	453.5 MIL LBS	T72	MISC CHEMS	18.1 MIL LBS
000071556	1,1,1-TRICHLOROETHANE (METHYLCHLOROFORM)	440.7 MIL LBS	T72	MISC CHEMS	284.5 MIL LBS
000075718	DICHLORODIFLUOROMETHANE	439.2 MIL LBS	T72	MISC CHEMS	401.9 MIL LBS
000117817	DI(2-ETHYLHEXYL)PHTHALATE	435.0 MIL LBS	T72	PLASTICIZERS	441.6 MIL LBS
000079016	TRICHLOROETHYLENE	426.7 MIL LBS	T72	MISC CHEMS	429.5 MIL LBS
000078922	SEC-BUTYL ALCOHOL	417.0 MIL LBS	SRI	MISC CHEMS	27.1 MIL LBS
000062533	ANILINE (ANILINE OIL)	409.8 MIL LBS	T72	CYCLIC INTERMED	
000108907	CHLOROBENZENE, MONO	403.5 MIL LBS	T72	CYCLIC INTERMED	
009010984	POLYCHLOROPRENE (NEOPRENE)	378.0 MIL LBS	SRI	ELASTOMERS	421.1 MIL LBS
000078795	ISOPRENE (2-METHYL-1,3-BUTADIENE)	372.7 MIL LBS	T72	CRUDE PRODUCTS	
025322694	POLYPROPYLENE GLYCOL	359.2 MIL LBS	T72	MISC CHEMS	26.6 MIL LBS
000106898	EPICHLOROHYDRIN	354.0 MIL LBS	SRI	MISC CHEMS	
000111466	DIETHYLENE GLYCOL	350.0 MIL LBS	SRI	MISC CHEMS	93.4 MIL LBS
009003296	POLYBUTENE	335.0 MIL LBS	T72	CRUDE PRODUCTS	333.3 MIL LBS
008061527	LIGNINSULFONIC ACID, CALCIUM SALT	326.6 MIL LBS	T72	SURF-ACTIV AGENT	329.9 MIL LBS
000106934	1,2-DIBROMOETHANE (ETHYLENE DIBROMIDE)	315.5 MIL LBS	T72	MISC CHEMS	304.4 MIL LBS
000074862	ACETYLENE	308.4 MIL LBS	T72	CRUDE PRODUCTS	
000075694	TRICHLOROFLUOROMETHANE	299.6 MIL LBS	T72	MISC CHEMS	274.1 MIL LBS
009003310	STEREO POLYISOPRENE	294.9 MIL LBS	T72	ELASTOMERS	269.7 MIL LBS
009010859	POLYISOBUTYLENE-ISOPRENE ELASTOMERS (BUTYL)	289.9 MIL LBS	T72	ELASTOMERS	251.0 MIL LBS
000140885	ETHYL ACRYLATE	275.3 MIL LBS	T72	MISC CHEMS	
000108316	MALEIC ANHYDRIDE	274.4 MIL LBS	T72	MISC CHEMS	
000080057	4,4'-ISOPROPYLIDENEDIPHENOL (BISPHENOL A)	255.2 MIL LBS	T72	CYCLIC INTERMED	
000067663	CHLOROFORM	234.7 MIL LBS	T72	MISC CHEMS	167.8 MIL LBS
000141786	ETHYL ACETATE, 85%	212.0 MIL LBS	T72	MISC CHEMS	156.1 MIL LBS
000108101	4-METHYL-2-PENTANONE (METHYL ISOBUTYL KETONE)	208.3 MIL LBS	T72	MISC CHEMS	201.0 MIL LBS
000110805	ETHYLENE GLYCOL MONOETHYL ETHER (2-ETHOXYETHANOL)	205.4 MIL LBS	T72	MISC CHEMS	197.5 MIL LBS
000119073	N-OCTYL N-DECYL PHTHALATE	200.6 MIL LBS	SRI	PLASTICIZERS	203.0 MIL LBS
009010791	ETHYLENE-PROPYLENE RUBBER	199.6 MIL LBS	T72	ELASTOMERS	169.5 MIL LBS
000056815	GLYCEROL, SYNTHETIC ONLY	199.2 MIL LBS	T72	MISC CHEMS	69.4 MIL LBS
000095807	TOLUENE-2,4-DIAMINE (4-M-TOLYLENEDIAMINE)	167.9 MIL LBS	T72	CYCLIC INTERMED	
000077929	CITRIC ACID	163.0 MIL LBS	SRI	MISC CHEMS	129.2 MIL LBS
009003183	POLYBUTADIENE-ACRYLONITRILE ELASTOMERS	159.7 MIL LBS	T72	ELASTOMERS	150.6 MIL LBS
000065850	BENZOIC ACID, TECH.	155.5 MIL LBS	T72	CYCLIC INTERMED	
026761400	DIISODECYL PHTHALATE	153.3 MIL LBS	T72	PLASTICIZERS	135.6 MIL LBS
027176870	DODECYLBENZENESULFONIC ACID	143.4 MIL LBS	SRI	SURF-ACTIV AGENT	
000075058	ACETONITRILE	135.0 MIL LBS	SRI	MISC CHEMS	69.5 MIL LBS
000111762	2-BUTOXYETHANOL (ETHYLENE GLYCOL MONOBUTYL ETHER)	133.3 MIL LBS	T72	MISC CHEMS	122.6 MIL LBS
000141322	BUTYL ACRYLATE	125.6 MIL LBS	T72	MISC CHEMS	
000079107	ACRYLIC ACID	123.2 MIL LBS	T72	MISC CHEMS	
000050704	SORBITOL	121.4 MIL LBS	T72	MISC CHEMS	52.2 MIL LBS
000109864	ETHYLENE GLYCOL MONOMETHYL ETHER	119.1 MIL LBS	T72	MISC CHEMS	29.4 MIL LBS
000115775	PENTAERYTHRITOL	110.1 MIL LBS	T72	MISC CHEMS	
001120043	OCTADECYL SULFATE, SODIUM SALT	110.0 MIL LBS	SRI	SURF-ACTIV AGENT	111.7 MIL LBS
001912249	ATRAZINE	< 110.0 MIL LBS	SRI	PESTICIDES	111.1 MIL LBS
009003547	STYRENE-ACRYLONITRILE RESINS	105.0 MIL LBS	T72	PLASTIC & RESIN	111.7 MIL LBS
000111422	2,2'-IMINODIETHANOL (DIETHANOLAMINE)	101.1 MIL LBS	T72	MISC CHEMS	26.0 MIL LBS
000102716	2,2',2''-NITRILOTRIETHANOL (TRIETHANOLAMINE)	100.7 MIL LBS	T72	MISC CHEMS	35.8 MIL LBS

Table 3-1 (continued)

025154523	NONYLPHENOL		100.3 MIL LBS	T72	CYCLIC INTERMED	
008001794	CASTOR OIL		100.0 MIL LBS	SRT	SURF-ACTIV AGENT	129.7 MIL LBS
000108781	MELAMINE		100.0 MIL LBS	SRI	CYCLIC INTERMED	
000078831	ISOBUTYL ALCOHOL (ISOPROPYL CARBINOL)		96.4 MIL LBS	T72	MISC CHEMS	29.5 MIL LBS
000124403	DIMETHYLAMINE		95.9 MIL LBS	T72	MISC CHEMS	26.6 MIL LBS
000123864	N-BUTYL ACETATE, UNMIXED		95.7 MIL LBS	T72	MISC CHEMS	97.1 MIL LBS
000100970	HEXAMETHYLENETETRAMINE		95.2 MIL LBS	T72	MISC CHEMS	60.4 MIL LBS
000112276	TRIETHYLENE GLYCOL		92.5 MIL LBS	SRI	MISC CHEMS	70.8 MIL LBS
009003207	POLYVINYL ACETATE RESINS		90.0 MIL LBS	T71	PLASTIC & RESIN	
008013078	EPOXIDIZED SOYA OILS		85.1 MIL LBS	T72	PLASTICIZERS	74.7 MIL LBS
000071238	PROPYL ALCOHOL (PROPANOL)		83.1 MIL LBS	T72	MISC CHEMS	63.6 MIL LBS
000141435	2-AMINOETHANOL (MONOETHANOLAMINE)		82.1 MIL LBS	T72	MISC CHEMS	29.3 MIL LBS
000100447	ALPHA-CHLOROTOLUENE (BENZYL CHLORIDE)		80.4 MIL LBS	T72	CYCLIC INTERMED	
009002895	POLYVINYL ALCOHOL		78.6 MIL LBS	T72	PLASTIC & RESIN	104.0 MIL LBS
000106467	P-DICHLOROBENZENE		77.3 MIL LBS	T72	CYCLIC INTERMED	70.7 MIL LBS
000060297	ETHYL ETHER, TECHNICAL		69.4 MIL LBS	T72	MISC CHEMS	55.7 MIL LBS
009000117	SODIUM CARBOXYMETHYLCELLULOSE, 100%		69.0 MIL LBS	T72	MISC CHEMS	71.0 MIL LBS
000064028	(ETHYLENEDINITRILO)TETRAACETIC ACID, TETRASODIUM SALT		66.3 MIL LBS	T72	MISC CHEMS	65.3 MIL LBS
000095501	O-DICHLOROBENZENE		62.4 MIL LBS	T72	CYCLIC INTERMED	27.1 MIL LBS
000106989	1-BUTENE		61.4 MIL LBS	T72	CRUDE PRODUCTS	
000107153	ETHYLENEDIAMINE		59.4 MIL LBS	SRI	MISC CHEMS	22.5 MIL LBS
000109999	TETRAHYDROFURAN		59.0 MIL LBS	SRI	CYCLIC INTERMED	42.2 MIL LBS
000079094	PROPIONIC ACID		56.0 MIL LBS	T72	MISC CHEMS	
001319773	CRESYLIC ACID, REFINED		55.0 MIL LBS	T72	CYCLIC INTERMED	30.4 MIL LBS
000063252	CARBARYL	<	55.0 MIL LBS	SRI	PESTICIDES	50.5 MIL LBS
000067481	CHOLINE CHLORIDE (ALL GRADES)		54.5 MIL LBS	T72	MEDICINAL CHEMS	56.1 MIL LBS
009002908	POLYETHYLENE GLYCOL		52.4 MIL LBS	T72	MISC CHEMS	31.8 MIL LBS
025265718	DIPROPYLENE GLYCOL		51.8 MIL LBS	T72	MISC CHEMS	
000110178	FUMARIC ACID		51.5 MIL LBS	T72	MISC CHEMS	10.2 MIL LBS
000298000	PHOSPHOROTHIOATE (METHYL PARATHION)		51.1 MIL LBS	T72	PESTICIDES	52.7 MIL LBS
001330785	TRICRESYL PHOSPHATE		50.2 MIL LBS	T72	PLASTICIZERS	43.4 MIL LBS
000107415	2-METHYL-2,4-PENTANEDIOL		50.0 MIL LBS	SRI	MISC CHEMS	50.6 MIL LBS
009004700	NITROCELLULOSE		50.0 MIL LBS	SRI	MISC CHEMS	51.5 MIL LBS
009003274	POLYISOBUTYLENE		50.0 MIL LBS	SRI	ELASTOMERS	51.5 MIL LBS
000108112	METHYL ISOBUTYL CARBINOL		50.0 MIL LBS	SRI	MISC CHEMS	40.8 MIL LBS
008001352	TOXAPHENE (CHLORINATED CAMPHENE)	<	50.0 MIL LBS	SRI	PESTICIDES	50.5 MIL LBS
000095487	O-CRESOL		49.7 MIL LBS	T72	CYCLIC INTERMED	15.6 MIL LBS
000087865	PENTACHLOROPHENOL (PCP)		49.7 MIL LBS	T72	PESTICIDES	
000142472	MONOSODIUM GLUTAMATE		47.3 MIL LBS	T72	FLAVOR & PERFUME	51.[illegible] MIL LBS
000069727	SALICYLIC ACID, TECH.		47.1 MIL LBS	T72	CYCLIC INTERMED	
000064186	FORMIC ACID		46.9 MIL LBS	T72	MISC CHEMS	24.1 MIL LBS
000075047	ETHYLAMINE, MONO		45.9 MIL LBS	SRI	MISC CHEMS	14.4 MIL LBS
000103117	2-ETHYL-1-HEXYL ACRYLATE		45.5 MIL LBS	T72	MISC CHEMS	
000050293	DDT		45.0 MIL LBS	SRI	PESTICIDES	42.5 MIL LBS
000103231	DI(2-ETHYLHEXYL)ADIPATE		44.9 MIL LBS	T72	PLASTICIZERS	39.4 MIL LBS
000111900	DIETHYLENE GLYCOL MONOETHYL ETHER		41.2 MIL LBS	T72	MISC CHEMS	36.6 MIL LBS
000087901	TRICHLOROISOCYANURIC ACID		40.0 MIL LBS	SRI	SURF-ACTIV AGENT	41.2 MIL LBS
000110441	SORBIC ACID		40.0 MIL LBS	SRI	MISC CHEMS	20.6 MIL LBS
025013154	VINYLTOLUENE		40.0 MIL LBS	SRI	CYCLIC INTERMED	12.0 MIL LBS
000094757	2,4-DICHLOROPHENOXYACETIC ACID (2,4-D)	<	40.0 MIL LBS	SRI	PESTICIDES	
025053489	POLYBUTADIENE-STYRENE-VINYLPYRIDINE ELASTOMERS		38.2 MIL LBS	T72	ELASTOMERS	39.3 MIL LBS
001592230	CALCIUM STEARATE		37.8 MIL LBS	SRT	SURF-ACTIV AGENT	38.9 MIL LBS
001300727	XYLENESULFONIC ACID, SODIUM SALT		37.4 MIL LBS	T72	SURF-ACTIV AGENT	40.5 MIL LBS
000050782	ASPIRIN		35.0 MIL LBS	T72	MEDICINAL CHEMS	35.9 MIL LBS
025167708	DIISOBUTYLENE (DIISOBUTENE)		35.0 MIL LBS	SRI	CRUDE PRODUCTS	
000126330	SULFOLANE		35.0 MIL LBS	SRT	PLASTICIZERS	35.5 MIL LBS
000122394	DIPHENYLAMINE		33.8 MIL LBS	T72	CYCLIC INTERMED	
001338245	NAPHTHENIC ACID		33.2 MIL LBS	T72	CRUDE PRODUCTS	
000074895	MONOMETHYLAMINE		33.1 MIL LBS	T72	MISC CHEMS	
000111400	DIETHYLENETRIAMINE		32.4 MIL LBS	T72	MISC CHEMS	16.7 MIL LBS
000109604	PROPYL ACETATE		32.4 MIL LBS	T72	MISC CHEMS	24.8 MIL LBS

Table 3-1 (continued)

027554263	DIISO-OCTYL PHTHALATE	32.3 MIL LBS	T72	PLASTICIZERS	32.8 MIL LBS
000141537	SODIUM FORMATE, TECH.	32.0 MIL LBS	SRI	MISC CHEMS	22.9 MIL LBS
000112356	TRIETHYLENE GLYCOL MONOMETHYL ETHER	31.7 MIL LBS	T72	MISC CHEMS	27.2 MIL LBS
000147477	1,2-DIHYDRO-2,2,4-TRIMETHYLQUINOLINE	30.0 MIL LBS	SRI	RUBBER-PROC CHEM	25.0 MIL LBS
000121755	MALATHION	30.0 MIL LBS	SRI	PESTICIDES	30.3 MIL LBS
009004620	HYDROXYETHYL CELLULOSE	30.0 MIL LBS	SRI	MISC CHEMS	22.9 MIL LBS
000084742	DIBUTYL PHTHALATE	29.1 MIL LBS	T72	PLASTICIZERS	29.5 MIL LBS
000075503	TRIMETHYLAMINE	28.8 MIL LBS	T72	MISC CHEMS	20.6 MIL LBS
000098839	ALPHA-METHYLSTYRENE	28.6 MIL LBS	T72	CYCLIC INTERMED	
031566311	GLYCEROL MONOSTEARATE	27.2 MIL LBS	T72	SURF-ACTIV AGENT	28.0 MIL LBS
007440213	SILICONE ELASTOMERS	26.0 MIL LBS	T72	ELASOTMERS	21.0 MIL LBS
000151213	DODECYL SULFATE, SODIUM SALT	26.8 MIL LBS	T72	SURF-ACTIV AGENT	27.6 MIL LBS
000057749	CHLORDAN	25.0 MIL LBS	SRI	PESTICIDES	25.3 MIL LBS
000309002	ALDRIN	25.0 MIL LBS	SRI	PESTICIDES	25.3 MIL LBS
000112345	DIETHYLENE GLYCOL MONOBUTYL ETHER	24.8 MIL LBS	T72	MISC CHEMS	25.1 MIL LBS
000074839	METHYL BROMIDE	24.6 MIL LBS	T72	PESTICIDES	22.4 MIL LBS
000119062	DITRIDECYL PHTHALATE	23.9 MIL LBS	T72	PLASTICIZERS	24.3 MIL LBS
000110918	MORPHOLINE	23.3 MIL LBS	T72	MISC CHEMS	12.4 MIL LBS
001918167	PROPACHLOR	23.0 MIL LBS	SRI	PESTICIDES	23.2 MIL LBS
002008391	2,4-DICHLOROPHENOXYACETIC ACID DIMETHYLAMINE SALT	22.5 MIL LBS	T72	PESTICIDES	
026249207	BUTYLENE OXIDE	22.0 MIL LBS	SRI	MISC CHEMS	
004075814	CALCIUM PROPIONATE	21.4 MIL LBS	T72	MISC CHEMS	22.0 MIL LBS
000120785	2,2'-DITHIOBIS(BENZOTHIAZOLE)	21.3 MIL LBS	T72	RUBBER PROC CHEMS	19.7 MIL LBS
000112276	TRIETHYLENE GLYCOL MONOETHYL ETHER	21.2 MIL LBS	T72	MISC CHEMS	21.5 MIL LBS
000133904	2,5-DICHLORO-3-AMINOBENZOIC ACID, AMMONIUM SALT (AMIBEN)	20.0 MIL LBS	SRT	PESTICIDES	20.2 MIL LBS
001582098	TRIFLURALIN	20.0 MIL LBS	SRI	PESTICIDES	20.2 MIL LBS
009004675	METHYL CELLULOSE	20.0 MIL LBS	SRI	MISC CHEMS	13.6 MIL LBS
000144194	2,2,4-TRIMETHYL-1,3-PENTANEDIOL	20.0 MIL LBS	SRI	PLASTICERS	16.3 MIL LBS
000557051	ZINC STEARATE	19.4 MIL LBS	T72	MISC CHEMS	20.0 MIL LBS
009003058	POLYACRYLAMIDE	19.1 MIL LBS	T72	MISC CHEMS	
000084662	DIETHYL PHTHALATE	19.0 MIL LBS	T72	PLASTICIZERS	19.3 MIL LBS
000127093	SODIUM ACETATE	18.1 MIL LBS	T71	MISC CHEMS	
000112243	TRIETHYLENETETRAMINE	18.0 MIL LBS	T72	MISC CHEMS	
000074884	IODOMETHANE (METHYL IODIDE)	18.0 MIL LBS	T72	MISC CHEMS	
000133062	N-TRICHLOROMETHYLTHIO-4-CYCLOHEXENE-1,2-DICARBOXIMIDE (CAPTAN)	18.0 MIL LBS	SRI	PESTICIDES	18.2 MIL LBS
000128370	2,6-DI-TERT-BUTYL-P-CRESOL, TECH.	17.8 MIL LBS	T72	MISC CHEMS	18.4 MIL LBS
000142847	DI-N-PROPYLAMINE	16.7 MIL LBS	T72	MISC CHEMS	
000111273	HEXYL ALCOHOL	16.3 MIL LBS	T72	MISC CHEMS	
000139968	DODECYL SULFATE, TRIETHANOLAMINE SALT	16.1 MIL LBS	T72	SURF-ACTIV AGENT	16.5 MIL LBS
000050817	VITAMIN C	15.6 MIL LBS	T72	MEDICINAL CHEMS	11.1 MIL LBS
000056382	PARATHION	15.0 MIL LBS	SRI	PESTICIDES	15.2 MIL LBS
009003014	POLYACRYLATE ELASTOMERS	15.0 MIL LBS	SRT	ELASTOMERS	15.5 MIL LBS
001643205	N,N'-DIMETHYLDODECYLAMINE OXIDE (LAURYL DIMETHYLAMINE OXIDE)	15.0 MIL LBS	SRI	SURF-ACTIV AGENT	15.5 MIL LBS
000080433	DICUMYL PEROXIDE	15.0 MIL LBS	SRI	RUBBER-PROC CHEM	15.3 MIL LBS
000095316	N-TERT-BUTYL-2-BENZOTHIAZOLESULFENAMIDE <	15.0 MIL LBS	SRI	RUBBER-PROC CHEM	
026444495	CRESYL DIPHENYL PHOSPHATE	14.6 MIL LBS	T72	PLASTICIZERS	
000108203	ISOPROPYL ETHER	14.0 MIL LBS	SRI	MISC CHEMS	14.2 MIL LBS
000123911	DIOXANE	13.8 MIL LBS	T72	MISC CHEMS	14.0 MIL LBS
000532321	BENZOIC ACID, SODIUM SALT	13.3 MIL LBS	T72	MISC CHEMS	
009002840	POLYTETRAFLUOROETHYLENE	13.3 MIL LBS	T72	PLASTIC & RESIN	15.0 MIL LBS
000137268	BIS(DIMETHYLTHIOCARBAMOYL) DISULFIDE	13.1 MIL LBS	T72	RUBBER PROC CHEMS	
000111773	DIETHYLENE GLYCOL MONOMETHYL ETHER	12.7 MIL LBS	SRI	MISC CHEMS	13.1 MIL LBS
000577117	SULFOSUCCINIC ACID, BIS(2-ETHYLHEXYL) ESTER, SODIUM SALT	12.4 MIL LBS	SRI	SURF-ACTIV AGENT	12.6 MIL LBS
001331584	DODECYLBENZENESULFONIC ACID, ISOPROPYLAMINE SALT	12.2 MIL LBS	SRI	SURF-ACTIV AGENT	
000081812	WARFARIN	12.0 MIL LBS	SRT	PESTICIDES	
008034002	GLYCEROL MONOESTER OF LARD ACIDS	12.0 MIL LBS	SRI	SURF-ACTIV AGENT	12.4 MIL LBS
000123319	HYDROQUINONE, TECH.	11.8 MIL LBS	T72	CYCLIC INTERMED	
000112607	TETRAETHYLENE GLYCOL	11.8 MIL LBS	T72	MISC CHEMS	
000103242	DI(2-ETHYLHEXYL)AZELATE	11.3 MIL LBS	T72	PLASTICIZERS	
000109897	DIETHYLAMINE	11.1 MIL LBS	T72	MISC CHEMS	
000115866	TRIPHENYL PHOSPHATE	10.6 MIL LBS	T72	PLASTICIZERS	

Table 3-1 (continued)

000100516	BENZYL ALCOHOL		10.4 MIL LBS	T72	FLAVOR & PERFUME	
000147148	PIGMENT BLUE 15, ALPHA AND BETA FORMS		10.4 MIL LBS	T72	ORG PIGMENTS	
012001762	VITAMIN B-COMPLEX		10.3 MIL LBS	T72	MEDICINAL CHEMS	12.9 MIL LBS
000096128	1,2-DIBROMO-3-CHLOROPROPANE (DBCP)		10.0 MIL LBS	SRI	PESTICIDES	
000072435	METHOXYCHLOR		10.0 MIL LBS	SRI	PESTICIDES	
000093710	2-CHLORO-N,N-DIALLYLACETAMIDE (CDAA)		10.0 MIL LBS	SRI	PESTICIDES	
000333415	DIAZINON		10.0 MIL LBS	SRI	PESTICIDES	
008013067	CASTOR OIL ACID, SODIUM SALT		10.0 MIL LBS	SRI	SURF-ACTIV AGENT	
008052504	TALLOW, SULFATED, SODIUM SALT		10.0 MIL LBS	T72	SURF-ACTIV AGENT	
000151213	2-ETHYLHEXYL SULFATE, SODIUM SALT		10.0 MIL LBS	SRI	SURF-ACTIV AGENT	
000103968	N,N'-BIS(1-METHYLHEPTYL)-P-PHENYLENEDIAMINE	<	10.0 MIL LBS	SRI	RUBBER PROC CHEMS	
000131113	DIMETHYL PHTHALATE		9.7 MIL LBS	T72	PLASTICIZERS	
002492264	2-BENZOTHIAZOLETHIOL, SODIUM SALT		9.7 MIL LBS	T72	CYCLIC INTERMED	
000105760	DIBUTYL MALEATE		9.6 MIL LBS	T72	MISC CHEMS	
000138863	DI-P-MENTHA-1,8-DIENE (LIMONENE)		9.3 MIL LBS	T72	CYCLIC INTERMED	
000128427	4,4'-DINITROSTILBENE-2,2'-DISULFONIC ACID		9.2 MIL LBS	T72	CYCLIC INTERMED	
001330865	DIISO-OCTYL ADIPATE		9.2 MIL LBS	T71	PLASTICIZERS	
014906979	GLUCONIC ACID, SODIUM SALT		8.9 MIL LBS	T72	MISC CHEMS	
000110292	N-OCTYL N-DECYL ADIPATE		8.8 MIL LBS	T72	PLASTICIZERS	
000095330	N-CYCLOHEXYL-2-BENZOTHIAZOLESULFENAMIDE		8.8 MIL LBS	T72	RUBBER PROC CHEMS	
000111411	2-(2-AMINOETHYLAMINO)ETHANOL		8.8 MIL LBS	T72	MISC CHEMS	
000069727	SALICYLIC ACID		8.7 MIL LBS	T72	MEDICINAL CHEMS	
000123955	N-BUTYL STEARATE		8.3 MIL LBS	T72	PLASTICIZERS	
000298044	DISULFOTON		8.0 MIL LBS	SRI	PESTICIDES	
000298022	O,O-DIETHYL S-(ETHYLTHIO)METHYL PHOSPHORODITHIOATE (PHORATE)		8.0 MIL LBS	SRI	PESTICIDES	
001563662	CARBOFURAN		8.0 MIL LBS	SRI	PESTICIDES	
000078784	ISOPENTANE		8.0 MIL LBS	T72	CRUDE PRODUCTS	
000121039	5-NITRO-O-TOLUENESULFONIC ACID (SO3H=1)		8.0 MIL LBS	T72	CYCLIC INTERMED	
000314409	5-BROMO-3-SEC-BUTYL-6-METHYLURACIL (BROMACIL)		8.0 MIL LBS	SRI	PESTICIDES	
008033985	GLYCEROL MONOESTER OF COTTONSEED OIL ACIDS		8.0 MIL LBS	SRI	SURF-ACTIV AGENT	
006033965	GLYCEROL MONOESTER OF COTTONSEED OIL ACIDS		8.0 MIL LBS	SRI	SURF-ACTIV AGENT	
000094360	BENZOYL PEROXIDE		7.6 MIL LBS	T72	MISC CHEMS	
000128370	2,6-DI-TERT-BUTYL-P-CRESOL		7.5 MIL LBS	T72	MISC CHEMS	
009000695	PECTIN		7.2 MIL LBS	SRI	MEDICINAL CHEMS	
000081118	4,4'-DIAMINO-2,2'-STILBENEDISULFONIC ACID		7.1 MIL LBS	T72	CYCLIC INTERMED	
027323417	DODECYLBENZENESULFONIC ACID, TRIETHANOLAMINE SALT		6.9 MIL LBS	T72	SURF-ACTIV AGENT	
001937377	DIRECT BLACK 38		6.7 MIL LBS	T72	DYES	
006358856	PIGMENT YELLOW 12		6.5 MIL LBS	T72	ORG PIGMENTS	
000142918	ISOPROPYL PALMITATE		6.5 MIL LBS	T72	PLASTICIZERS	
000142165	DIOCTYL MALEATE		6.3 MIL LBS	T72	MISC CHEMS	
000076448	HEPTACHLOR		6.0 MIL LBS	SRI	PESTICIDES	
001918009	3,6-DICHLORO-2-ANISIC ACID (DICAMBA)		6.0 MIL LBS	SRI	PESTICIDES	
000330541	3-(3,4-DICHLOROPHENYL)-1,1-DIMETHYL UREA (DIURON)		6.0 MIL LBS	SRI	PESTICIDES	
002008415	ETHYL-N,N-DIISOBUTYL THIOLCARBAMATE		6.0 MIL LBS	SRI	PESTICIDES	
000709988	PROPANIL		6.0 MIL LBS	SRI	PESTICIDES	
000149304	2-MERCAPTOBENZOTHIAZOLE		6.0 MIL LBS	T72	RUBBER PROC CHEMS	
000119368	METHYL SALICYLATE		5.8 MIL LBS	T72	FLAVOR & PERFUME	
000136607	BUTYL BENZOATE		5.6 MIL LBS	T72	MISC CHEMS	
000112163	LAUROYL CHLORIDE		5.5 MIL LBS	T72	MISC CHEMS	
009004993	POLYETHYLENE GLYCOL MONOSTEARATE		5.4 MIL LBS	T72	SURF-ACTIV AGENT	
000127082	POTASSIUM ACETATE		5.2 MIL LBS	T72	MISC CHEMS	
000124414	SODIUM METHOXIDE (SODIUM METHYLATE)		5.2 MIL LBS	T72	MISC CHEMS	
030526228	TOLUENESULFONIC ACID, POTASSIUM SALT		5.0 MIL LBS	SRI	SURF-ACTIV AGENT	
000759944	ETHYL N,N-DIPROPYLTHIOLCARBAMATE (EPTC)		5.0 MIL LBS	SRI	PESTICIDES	
000657841	TOLUENESULFONIC ACID, SODIUM SALT		5.0 MIL LBS	SRI	SURF-ACTIV AGENT	
000127208	2,2-DICHLOROPROPIONIC ACID, SODIUM SALT (DALAPON)		5.0 MIL LBS	SRI	PESTICIDES	
000122349	2-CHLORO-4,6-BIS(ETHYLAMINO)-S-TRIAZINE (SIMAZINE)		5.0 MIL LBS	SRI	PESTICIDES	
010124659	LAURIC ACID, POTASSIUM SALT		5.0 MIL LBS	SRI	SURF-ACTIV AGENT	
000078488	S,S,S-TRIBUTYL PHOSPHOROTRITHIOATE		5.0 MIL LBS	SRI	PESTICIDES	
002921882	O,O-DIETHYL O-3,5,6-TRICHLORO-2-PYRIDYL PHOSPHOROTHIOATE		5.0 MIL LBS	SRI	PESTICIDES	
000097392	1,3-DI-O-TOLYLGUANIDINE		5.0 MIL LBS	SRI	RUBBER-PROC CHEM	

Table 3-1 (continued)

000102067	1,3-DIPHENYLGUANIDINE		5.0 MIL LBS	SRI	RUBBER-PROC CHEM
000093765	2,4,5-TRICHLOROPHENOXYACETIC ACID ESTERS & SALTS	<	5.0 MIL LBS	SRI	PESTICIDES
001338234	2-BUTANONE PEROXIDE		4.8 MIL LBS	T72	MISC CHEMS
000110270	ISOPROPYL MYRISTATE		4.8 MIL LBS	T72	PLASTICIZERS
000081072	SACCHARIN		4.8 MIL LBS	SRI	FLAVOR & PERFUME
000557040	MAGNESIUM STEARATE		4.8 MIL LBS	T72	MISC CHEMS
000128041	DIMETHYLDITHIOCARBAMIC ACID, SODIUM SALT		4.6 MIL LBS	T72	RUBBER PROC CHEMS
001103364	PIGMENT RED 49, BARIUM TONER		4.6 MIL LBS	T72	ORG PIGMENTS
000100527	BENZALDEHYDE, TECH.		4.6 MIL LBS	T72	CYCLIC INTERMED
000109433	DIBUTYL SEBACATE		4.5 MIL LBS	T72	PLASTICIZERS
0[illegible]0586131	PIGMENT BLUE 19		4.5 MIL LBS	T72	ORG PIGMENTS
000090028	SALICYLALDEHYDE		4.5 MIL LBS	T72	CYCLIC INTERMED
000123331	1,2-DIHYDROPYRIDAZINE-3,6-DIONE (MALEIC HYDRAZIDE)		4.5 MIL LBS	T72	PESTICIDES
000135866	N-PHENYL-2-NAPHTHYLAMINE		4.5 MIL LBS	T72	RUBBER PROC CHEMS
000084617	DICYCLOHEXYL PHTHALATE		4.5 MIL LBS	T70	PLASTICIZERS
009005076	POLYETHYLENE GLYCOL DIOLEATE		4.4 MIL LBS	T72	SURF-ACTIV AGENT
000078115	PENTAERYTHRITOL TETRANITRATE		4.1 MIL LBS	T72	MISC CHEMS
000137406	SODIUM PROPIONATE		4.1 MIL LBS	T72	MISC CHEMS
000121335	VANILLIN, SYNTHETIC		4.0 MIL LBS	SRI	FLAVOR & PERFUME
000109739	MONO-N-BUTYLAMINE		4.0 MIL LBS	T72	MISC CHEMS
000155044	2-MERCAPTOBENZOTHIAZOLE, ZINC SALT		4.0 MIL LBS	T72	RUBBER PROC CHEMS
000086500	AZINPHOSMETHYL		4.0 MIL LBS	SRI	PESTICIDES
000115322	4,4'-DICHLORO-ALPHA-TRICHLOROMETHYLBENZHYDROL (DICOFOL)		4.0 MIL LBS	SRI	PESTICIDES
000136361	DIBUTYLDITHIOCARBAMIC ACID, ZINC SALT		4.0 MIL LBS	T72	RUBBER PROC CHEMS
002164172	FLUOMETURON		4.0 MIL LBS	SRI	PESTICIDES
000115902	O,O-DIETHYL O-P-(METHYLSULFINYL)PHENYL PHOSPHOROTHIOATE		4.0 MIL LBS	SRI	PESTICIDES
000096695	4,4'-THIOBIS(6-TERT-BUTYL-M-CRESOL)		4.0 MIL LBS	SRI	RUBBER-PROC CHEM
000077623	2,2'-METHYLENEBIS(6-(1-METHYLCYCLOHEXYL)-P-CRESOL)		4.0 MIL LBS	SRI	RUBBER-PROC CHEM
000085609	4,4'-BUTYLIDENEBIS(6-TERT-BUTYL-M-CRESOL)		4.0 MIL LBS	SRI	RUBBER-PROC CHEM
000111922	DI-N-BUTYLAMINE		3.8 MIL LBS	T72	MISC CHEMS
000137166	N-LAUROYLSARCOSINE, SODIUM SALT		3.8 MIL LBS	T72	SURF-ACTIV AGENT
009004813	POLYETHYLENE GLYCOL MONOLAURATE		3.8 MIL LBS	T72	SURF-ACTIV AGENT
000110850	PIPERAZINE		3.6 MIL LBS	T72	MEDICINAL CHEMS
000091667	N,N-DIETHYLANILINE		3.6 MIL LBS	T72	CYCLIC INTERMED
009004960	POLYETHYLENE GLYCOL MONO-OLEATE		3.6 MIL LBS	T72	SURF-ACTIV AGENT
003564214	PIGMENT RED 48		3.5 MIL LBS	T72	ORG PIGMENTS
000108010	2-DIMETHYLAMINOETHANOL		3.5 MIL LBS	T72	MISC CHEMS
000122623	DI(2-ETHYLHEXYL) SEBACATE		3.5 MIL LBS	T72	PLASTICIZERS
000136527	COBALT 2-ETHYLHEXOATE		3.4 MIL LBS	T72	MISC CHEMS
001321740	DIVINYLBENZENE		3.4 MIL LBS	T72	CYCLIC INTERMED
000129099	VAT YELLOW 2		3.3 MIL LBS	T72	DYES
001328536	PIGMENT GREEN 7		3.3 MIL LBS	T72	ORG PIGMENTS
000103844	ACETANILIDE, TECH.		3.2 MIL LBS	T72	CYCLIC INTERMED
000112629	METHYL OLEATE		3.1 MIL LBS	T72	PLASTICIZERS
0000900[illegible]0	O-ANISIDINE		3.1 MIL LBS	T72	CYCLIC INTERMED
000093721	2-(2,4,5-TRICHLOROPHENOXY)PROPIONIC ACID (SILVEX)		3.0 MIL LBS	SRI	PESTICIDES
000142314	OCTYL SULFATE, SODIUM SALT		3.0 MIL LBS	SRI	SURF-ACTIV AGENT
000944229	O-ETHYL S-PHENYLETHYL PHOSPHORODITHIOATE		3.0 MIL LBS	SRI	PESTICIDES
000563122	ETHION		3.0 MIL LBS	SRI	PESTICIDES
000082688	PENTACHLORONITROBENZENE (PCNB)		3.0 MIL LBS	SRI	PESTICIDES
000957517	N,N-DIMETHYL-2,2-DIPHENYLACETAMIDE		3.0 MIL LBS	SRI	PESTICIDE
000088857	DINITROBUTYLPHENOL (DNBP)		3.0 MIL LBS	SRI	PESTICIDES
00[illegible]026639	TRIDECYL SULFATE, SODIUM SALT		3.0 MIL LBS	SRI	SURF-ACTIV AGENT
002439103	N-DODECYLGUANIDINE ACETATE (DODINE)	<	3.0 MIL LBS	SRI	PESTICIDES
000130201	VAT BLUE 6		2.9 MIL LBS	T72	DYES
000059029	VITAMIN E		2.9 MIL LBS	T72	MEDICINAL CHEMS
025496724	GLYCEROL MONO-OLEATE		2.8 MIL LBS	T72	SURF-ACTIV AGENT
00[illegible]42530	DIISODECYL ADIPATE		2.8 MIL LBS	T72	PLASTICIZERS
002832408	DIRECT YELLOW [illegible]		2.8 MIL LBS	T72	DYES
005160021	PIGMENT RED 53, BARIUM TONER		2.8 MIL LBS	T72	ORG PIGMENTS
000300925	ALUMINUM DISTEARATE		2.7 MIL LBS	T72	MISC CHEMS

Table 3-1 (continued)

000104461	P-PROPENYLANISOLE (ANETHOLE)	2.7 MIL LBS	T72	FLAVOR & PERFUME
000097745	BIS(DIMETHYLTHIOCARBAMOYL) SULFIDE	2.6 MIL LBS	T72	RUBBER PROC CHEMS
001323393	1,2-PROPANEDIOL MONOSTEARATE	2.6 MIL LBS	T72	SURF-ACTIV AGENT
000142778	BUTYL OLEATE	2.4 MIL LBS	T72	PLASTICIZERS
001325377	DIRECT YELLOW 11	2.4 MIL LBS	T72	DYES
000137304	DIMETHYLDITHIOCARBAMIC ACID	2.4 MIL LBS	T72	RUBBER PROC CHEMS
026264051	DODECYLBENZENESULFONIC ACID, ISOPROPYLAMINE SALT	2.2 MIL LBS	T72	SURF-ACTIV AGENT
001338029	NAPHTHENIC ACID, COPPER SALT	2.2 MIL LBS	T72	PESTICIDES
002425856	PIGMENT RED 3	2.1 MIL LBS	T72	ORG PIGMENTS
000081641	1,4-DIHYDROXYANTHRAQUINONE (QUINIZARIN)	2.1 MIL LBS	T72	CYCLIC INTERMED
005468757	PIGMENT YELLOW 14	2.1 MIL LBS	T72	ORG PIGMENTS
000075605	DIMETHYLARSENIC ACID (CACODYLIC ACID)	2.0 MIL LBS	SRI	PESTICIDES
000104154	TOLUENESULFONIC ACID	2.0 MIL LBS	SRI	SURF-ACTIV AGENT
000133073	N-TRICHLOROMETHYLTHIOPHTHALIMIDE (FOLPET)	2.0 MIL LBS	SRI	PESTICIDES
000299843	DIMETHYL 2,4,5-TRICHLOROPHENYL PHOSPHOROTHIONATE (RONNEL)	2.0 MIL LBS	SRI	PESTICIDES
000143077	LAURIC ACID	2.0 MIL LBS	T72	SURF-ACTIV AGENT
000786196	S-(((P-CHLOROPHENYL)THIO)METHYL) O,O-DIETHYL PHOSPHORODITHIOATE	2.0 MIL LBS	SRI	PESTICIDES
001929777	S-PROPYL DIPROPYLTHIOCARBAMATE (VERNOLATE)	2.0 MIL LBS	SRI	PESTICIDES
000300765	1,2-DIBROMO-2,2-DICHLOROETHYL DIMETHYL PHOSPHATE (NALED)	2.0 MIL LBS	SRI	PESTICIDES
000115297	ENDOSULFAN	2.0 MIL LBS	SRI	PESTICIDES
000510156	CHLOROBENZILATE	2.0 MIL LBS	SRI	PESTICIDES
010213782	N,N-BIS(2-HYDROXYETHYL)OCTADECYLAMINE	2.0 MIL LBS	SRI	SURF-ACTIV AGENT
000086306	N-NITROSODIPHENYLAMINE	2.0 MIL LBS	T72	RUBBER PROC CHEMS
000330552	3-(3,4-DICHLOROPHENYL)-1-METHOXY-1-METHYLUREA	2.0 MIL LBS	SRI	PESTICIDES
004726141	4-(METHYLSULFONYL)-2,6-DINITRO-N,N-DIPROPYLANILINE (NITRALIN)	2.0 MIL LBS	SRI	PESTICIDES
000129679	ENDOTHALL	2.0 MIL LBS	SRI	PESTICIDES
001861321	DIMETHYL-2,3,5,6-TETRACHLOROTEREPHTHALATE (DCPA)	2.0 MIL LBS	SRI	PESTICIDE
000101213	ISOPROPYL N-(3-CHLOROPHENYL) CARBAMATE (CIPC)	2.0 MIL LBS	SRI	PESTICIDES
002939802	CAPTAFOL	2.0 MIL LBS	SRI	PESTICIDES
000515424	BENZENESULFONIC ACID, SODIUM SALT	2.0 MIL LBS	SRI	SURF-ACTIV AGENT
000060515	DIMETHOATE	2.0 MIL LBS	SRI	PESTICIDES
000546265	PIGMENT RED 90	1.9 MIL LBS	T72	ORG PIGMENTS
000103695	N-ETHYLANILINE, REFINED	1.9 MIL LBS	T72	CYCLIC INTERMED
014324551	DIETHYLDITHIOCARBAMIC ACID	1.9 MIL LBS	T72	RUBBER PROC CHEMS
012239348	DISPERSE BLUE 79	1.9 MIL LBS	T71	DYES
000128585	VAT GREEN 1	1.8 MIL LBS	T72	DYES
000074317	N,N'-DIPHENYL-P-PHENYLENEDIAMINE	1.8 MIL LBS	T72	RUBBER PROC CHEMS
000110054	TERT-BUTYL PEROXIDE (DI-TERT-BUTYL PEROXIDE)	1.8 MIL LBS	T72	MISC CHEMS
004208804	BASIC YELLOW 11	1.7 MIL LBS	T72	DYES
000100743	4-ETHYLMORPHOLINE	1.6 MIL LBS	T72	MISC CHEMS
026062782	PHENOL, STYRENATED	1.6 MIL LBS	T72	RUBBER PROC CHEMS
000104552	CINNAMALDEHYDE	1.6 MIL LBS	T72	FLAVOR & PERFUME
001323859	DISTEARYL 3,3'-THIODIPROPIONATE	1.6 MIL LBS	T72	MISC CHEMS
004404437	FLUORESCENT BRIGHTENING AGENT 28	1.6 MIL LBS	T72	DYES
005858822	PIGMENT RED 52	1.6 MIL LBS	T72	ORG PIGMENTS
002650182	ACID BLUE 9	1.5 MIL LBS	T72	DYES
005281049	PIGMENT RED 57, CALCIUM TONER	1.5 MIL LBS	T72	ORG PIGMENTS
000124237	N,N-DIMETHYLOCTADECYLAMINE	1.5 MIL LBS	SRI	SURF-ACTIV AGENT
000124287	N,N-DIMETHYLOCTADECYLAMINE	1.5 MIL LBS	T72	SURF-ACTIV AGENT
000143180	OLEIC ACID, POTASSIUM SALT	1.5 MIL LBS	T72	SURF-ACTIV AGENT
000140114	BENZYL ACETATE	1.4 MIL LBS	T72	FLAVOR & PERFUME
008016760	SPERM OIL, SULFATED, SODIUM SALT	1.4 MIL LBS	T72	SURF-ACTIV AGENT
003271769	VAT GREEN 3	1.4 MIL LBS	T72	DYES
000123284	DILAURYL 3,3'-THIODIPROPIONATE	1.4 MIL LBS	T72	MISC CHEMS
007549420	CALCIUM NAPHTHENATE	1.4 MIL LBS	T72	MISC CHEMS
000141173	DI(2-(2-BUTOXYETHOXY)ETHYL) ADIPATE	1.3 MIL LBS	T72	PLASTICIZERS
001103395	PIGMENT RED 49, CALCIUM TONER	1.3 MIL LBS	T72	ORG PIGMENTS
002475469	DISPERSE BLUE 3	1.3 MIL LBS	T72	DYES
000106241	3,7-DIMETHYL-TRANS-2,6-OCTADIEN-1-OL (GERANIOL)	1.2 MIL LBS	T72	FLAVOR & PERFUME
000136538	ZINC 2-ETHYLHEXANOATE	1.2 MIL LBS	T72	MISC CHEMS
000082053	7H-BENZ(DE)ANTHRACEN-7-ONE (BENZANTHRONE)	1.2 MIL LBS	T72	CYCLIC INTERMED

Table 3-1 (continued)

009005021	POLYETHYLENE GLYCOL DILAURATE	1.2 MIL LBS	T72	SURF-ACTIV AGENT
008004873	BASIC VIOLET 1	1.2 MIL LBS	T72	DYES
006250233	DISPERSE YELLOW 23	1.2 MIL LBS	T71	DYES
000121471	METANILIC ACID (M-AMINOBENZENESULFONIC ACID)	1.1 MIL LBS	T72	CYCLIC INTERMED
001934210	FD&C YELLOW NO 5	1.1 MIL LBS	T72	DYES
010401500	DIRECT BLUE 218	1.1 MIL LBS	T72	DYES
000123115	P-ANISALDEHYDE	1.1 MIL LBS	T72	FLAVOR & PERFUMI
000068268	VITAMIN A	1.0 MIL LBS	T72	MEDICINAL CHEMS
003383968	O,O,O',O'-TETRAMETHYL O,O'-THIODI-P-PHENYLENE PHOSPHOROTHIOATE	1.0 MIL LBS	SRI	PESTICIDES
000134623	N,N-DIETHYLTOLUAMIDE (DEET)	1.0 MIL LBS	SRI	PESTICIDES
000124221	DODECYLAMINE	1.0 MIL LBS	SRI	SURF-ACTIV AGENT
002429734	DIRECT BLUE 2	1.0 MIL LBS	T72	DYES
000081492	1-AMINO-2,4-DIBROMOANTHRAQUINONE	1.0 MIL LBS	T72	CYCLIC INTERMED
009003014	POLYACRYLIC ACID	1.0 MIL LBS	T72	MISC CHEMS
006358312	PIGMENT YELLOW 74	1.0 MIL LBS	T72	ORG PIGMENTS
000051036	PIPERONYL BUTOXIDE	1.0 MIL LBS	SRI	PESTICIDES
000915673	FD&C RED NO 2	1.0 MIL LBS	T71	DYES
002783940	FD&C YELLOW NO 6	1.0 MIL LBS	T71	DYES

Table 3-2. INDUSTRIAL CHEMICALS WITHOUT CAS NUMBERS

NAME	PRODUCTION	SOURCE	USE CATEGORY	RELEASE POTENTIAL
XYLENES (MIXED TOTAL)	5600.0 MIL LBS	SRI	TAR & TAR CRUDES	904.6 MIL LBS
POLYETHYLENE & COPOLYMERS, DENSITY <0.940 (THERMOPLASTIC)	5360.3 MIL LBS	T72	PLASTIC & RESIN	5128.4 MIL LBS
POLYETHYLENE & COPOLYMERS, DENSITY >0.940 (THERMOPLASTIC)	2295.9 MIL LBS	T72	PLASTIC & RESIN	2079.7 MIL LBS
POLYSTYRENE, RUBBER-MODIFIED (THERMOPLASTIC)	1647.0 MIL LBS	T72	PLASTIC & RESIN	1727.4 MIL LBS
NYLON 6 AND 66 (POLYMERS FOR FIBER ONLY)	1547.2 MIL LBS	T72	MISC CHEMS	1552.1 MIL LBS
ACRYLIC RESINS	1000.0 MIL LBS	SRI	PLASTIC & RESIN	1101.6 MIL LBS
POLYACRYLONITRILE (FIBERS)	1000.0 MIL LBS	SRI	MISC CHEMS	988.7 MIL LBS
TETRAETHYLLEAD, TETRAMETHYLLEAD & OTHER ORGANOLEAD COMPOUNDS	972.5 MIL LBS	T72	MISC CHEMS	914.2 MIL LBS
UNSATURATED POLYESTER RESINS, TOTAL	950.0 MIL LBS	SRI	PLASTIC & RESIN	954.6 MIL LBS
POLYESTER RESINS (THERMOSETTING), TOTAL	930.4 MIL LBS	T72	PLASTIC & RESIN	
GLYCEROL TRI(POLYOXYPROPYLENE) ETHER	768.0 MIL LBS	SRI	MISC CHEMS	
ACRYLIC RESINS	758.6 MIL LBS	T72	PLASTIC & RESIN	
1-BUTENE & 2-BUTENE MIXTURES	752.8 MIL LBS	T72	CRUDE PRODUCTS	
HEXAMETHYLENEDIAMMONIUM ADIPATE (NYLON SALT)	719.6 MIL LBS	T72	MISC CHEMS	
ALKYD RESINS, PHTHALIC ANHYDRIDE TYPE (THERMOSETTING)	597.2 MIL LBS	T72	PLASTIC & RESIN	566.5 MIL LBS
BUTADIENE AND BUTYLENE FRACTIONS	566.0 MIL LBS	T72	CRUDE PRODUCTS	
ALKYLBENZENES	524.0 MIL LBS	T72	CYCLIC INTERMED	
POLYVINYL ACETATE, LATEXES (THERMOPLASTIC)	450.0 MIL LBS	SRI	PLASTIC & RESIN	
MIXED ALCOHOLS, C10 AND HIGHER	446.0 MIL LBS	T72	MISC CHEMS	38.2 MIL LBS
2,4(AND 2,6)-DINITROTOLUENE	433.9 MIL LBS	T72	CYCLIC INTERMED	
TOLUENE 2,4- AND 2,6-DIISOCYANATE (80/20 MIXTURE)	414.4 MIL LBS	T72	CYCLIC INTERMED	
LUBRICATING OIL & GREASE ADDITIVES	388.1 MIL LBS	SRI	MISC CHEMS	
NONENE (TRIPROPYLENE)	341.6 MIL LBS	T72	CRUDE PRODUCTS	
HEXANES & OTHER C6 HYDROCARBONS	339.7 MIL LBS	T72	CRUDE PRODUCTS	343.1 MIL LBS
MIXED LINEAR ALCOHOLS, ETHOXYLATED	323.7 MIL LBS	T72	SURF-ACTIV AGENT	328.6 MIL LBS
PENTENES, MIXED	319.0 MIL LBS	T72	CRUDE PRODUCTS	
CELLULOSIC PLASTICS & RESINS (THERMOPLASTIC)	256.8 MIL LBS	T72	PLASTIC & RESIN	234.8 MIL LBS
TETRAPROPYLENE	210.2 MIL LBS	T72	CRUDE PRODUCTS	
TALLOW ACIDS, POTASSIUM SALT	200.0 MIL LBS	SRI	SURF-ACTIV AGENT	206.0 MIL LBS
NONYLPHENOL, ETHOXYLATED	177.9 MIL LBS	T72	SURF-ACTIV AGENT	180.6 MIL LBS
EPOXY RESINS, UNMODIFIED TOTAL (THERMOSETTING)	176.0 MIL LBS	T72	PLASTIC & RESIN	129.7 MIL LBS
STYRENE POLYMERS, ALL OTHER	157.0 MIL LBS	SRI	PLASTIC & RESIN	141.7 MIL LBS
ISODECYL ALCOHOL	147.0 MIL LBS	T72	MISC CHEMS	75.7 MIL LBS
SUCROSE OCTA(POLYPROPOXYLENE)ETHER	140.0 MIL LBS	SRI	MISC CHEMS	128.1 MIL LBS
OIL-SOLUBLE PETROLEUM SULFONATE, CALCIUM SALT	139.5 MIL LBS	T72	MISC CHEMS	
COCONUT OIL ACIDS, SODIUM SALT	131.1 MIL LBS	T72	SURF-ACTIV AGENT	135.1 MIL LBS
POLYAMIDE RESINS, NYLON TYPE (THERMOPLASTIC)	123.0 MIL LBS	T72	PLASTIC & RESIN	111.7 MIL LBS
POLYESTER RESINS, SATURATED (THERMOPLASTIC)	115.0 MIL LBS	T72	PLASTIC & RESIN	
MIXED LINEAR ALCOHOLS, ETHOXYLATED & SULFATED, AMMONIUM SALT	103.8 MIL LBS	T72	SURF-ACTIV AGENT	105.4 MIL LBS
POLYSULFIDE ELASTOMERS	100.0 MIL LBS	SRI	ELASTOMERS	
POLYURETHANE & DIISOCYANATE RESINS	99.4 MIL LBS	T72	PLASTIC & RESIN	102.4 MIL LBS
ACETAL RESINS (THERMOPLASTIC)	95.4 MIL LBS	SRI	PLASTIC & RESIN	65.5 MIL LBS
ROSIN MODIFICATIONS, ALL OTHER (THERMOPLASTIC)	92.4 MIL LBS	T72	PLASTIC & RESIN	92.4 MIL LBS
THERMOSETTING RESINS	90.8 MIL LBS	T72	PLASTIC & RESIN	93.5 MIL LBS
NITRILOTRIACETIC ACID, TRISODIUM SALT	85.0 MIL LBS	SRI	MISC CHEMS	14.3 MIL LBS
HEPTENES, MIXED	83.8 MIL LBS	T72	CRUDE PRODUCTS	
SILICONE FLUIDS	74.7 MIL LBS	T72	MISC CHEMS	75.2 MIL LBS
ACYCLIC PHOSPHORODITHIOATE LUBRICATING OIL ADDITIVES	67.0 MIL LBS	T72	MISC CHEMS	68.6 MIL LBS
ISO-OCTYL ALCOHOLS	65.2 MIL LBS	T72	MISC CHEMS	15.8 MIL LBS
POLYPHENYLENE OXIDE-TYPE RESIN	63.0 MIL LBS	SRI	PLASTIC & RESIN	64.9 MIL LBS
POLYCARBONATE RESINS (THERMOPLASTIC)	61.5 MIL LBS	SRI	PLASTIC & RESIN	62.1 MIL LBS

Table 3-2 (continued)

LIGNINSULFONIC ACID, FERROCHROME SALT		60.0 MIL LBS	SRI	SURF-ACTIV AGENT	60.6 MIL LBS
1,3-DICHLOROPROPENE, 1,2-DICHLOROPROPANE		60.0 MIL LBS	SRI	MISC CHEMS	56.0 MIL LBS
LIGNINSULFONIC ACID, SODIUM SALT		58.7 MIL LBS	T72	SURF-ACTIV AGENT	59.3 MIL LBS
POLYURETHANE ELASTOMERS		57.3 MIL LBS	T72	ELASTOMERS	54.0 MIL LBS
CHLORINATED PARAFFINS, 35-64% CHLORINE		48.6 MIL LBS	T72	MISC CHEMS	50.3 MIL LBS
MIXED ALCOHOLS, C9 AND LOWER		44.9 MIL LBS	T72	MISC CHEMS	12.6 MIL LBS
MIXED ALCOHOLS, C6-C12 AND OTHERS		43.6 MIL LBS	T72	MISC CHEMS	22.5 MIL LBS
EPOXY RESINS, MODIFIED (THERMOSETTING)		43.2 MIL LBS	T72	PLASTIC & RESIN	35.0 MIL LBS
ESTERS, AMINES & SALTS OF 2,4-DICHLOROPHENOXYACETIC ACID		43.0 MIL LBS	SRI	PESTICIDES	43.4 MIL LBS
OIL-SOLUBLE PETROLEUM SULFONATE, SODIUM SALT		42.0 MIL LBS	T72	MISC CHEMS	
ACYCLIC DITHIOCARBAMIC ACID SALT FUNGICIDES		41.4 MIL LBS	T72	PESTICIDES	38.0 MIL LBS
LIGNINSULFONIC ACID, AMMONIUM SALT		40.0 MIL LBS	SRI	SURF-ACTIV AGENT	40.4 MIL LBS
ACYCLIC XANTHIC ACID SALTS		39.6 MIL LBS	T71	MISC CHEMS	
ALKYD RESINS, POLYBASIC ACID TYPE (THERMOSETTING)		38.7 MIL LBS	T72	PLASTIC & RESIN	39.9 MIL LBS
PINENE (ALPHA & BETA)		38.1 MIL LBS	T72	MISC CHEMS	
ROSIN & ROSIN ESTERS, UNMODIFIED (THERMOPLASTIC)		36.0 MIL LBS	T72	PLASTIC & RESIN	35.5 MIL LBS
DODECYL & TETRADECYL ALCS, ETHOXYLATED & SULFATED, NH4,NA		35.0 MIL LBS	SRI	SURF-ACTIV AGENT	36.1 MIL LBS
BIS-(HYDROGENATED TALLOW ALKYL) DIMETHYLAMMONIUM CHLORIDE		31.4 MIL LBS	T72	SURF-ACTIV AGENT	37.3 MIL LBS
OCTYL EPOXYTALLATES		31.4 MIL LBS	T72	PLASTICIZERS	32.0 MIL LBS
METHANEARSONIC ACID SALTS		30.7 MIL LBS	T72	PESTICIDES	31.0 MIL LBS
ACYCLIC PHOSPHORIC ACID ESTER PLASTICIZERS		29.4 MIL LBS	T72	PLASTICIZERS	25.9 MIL LBS
VAT BLUE DYES		26.5 MIL LBS	T72	DYES	35.6 MIL LBS
(M,P) CRESOL		28.3 MIL LBS	T72	CYCLIC INTERMED	
POLYAMIDE RESINS, NON-NYLON TYPE (THERMOPLASTIC)		27.3 MIL LBS	T72	PLASTIC & RESIN	25.4 MIL LBS
FLUORESCENT BRIGHTENING AGENTS ALL (EXCEPT FBA-28)		25.7 MIL LBS	SRI	DYES	25.5 MIL LBS
COCONUT OIL ACIDS, DIETHANOLAMINE CONDENSATE (AMINE/ACID=1/1)		21.5 MIL LBS	T72	SURF-ACTIV AGENT	22.1 MIL LBS
DINONYLPHENOL, ETHOXYLATED		20.0 MIL LBS	SRI	SURF-ACTIV AGENT	20.6 MIL LBS
2-ETHYLHEXANOL, ETHOXYLATED AND SULFATED, SODIUM SALT		20.0 MIL LBS	SRI	SURF-ACTIV AGENT	20.6 MIL LBS
2,4,5-TRICHLOROPHENOL ACID & SALTS		20.0 MIL LBS	SRI	PESTICIDES	20.2 MIL LBS
ISO-OCTYLPHENOL, ETHOXYLATED		20.0 MIL LBS	SRI	SURF-ACTIV AGENT	20.6 MIL LBS
(MIXED ALKYL)PHENOL, ETHOXYLATED		20.0 MIL LBS	SRI	SURF-ACTIV AGENT	20.6 MIL LBS
PHENOL, ETHOXYLATED		20.0 MIL LBS	SRI	SURF-ACTIV AGENT	20.0 MIL LBS
NONYL PHENYL PHOSPHITES, MIXED		20.0 MIL LBS	T72	RUBBER-PROC CHEM	20.3 MIL LBS
TALL OIL ACIDS, POTASSIUM SALT		19.5 MIL LBS	T72	SURF-ACTIV AGENT	20.1 MIL LBS
STEARIC ACID-ETHYLENEDIAMINE CONDENSATE		18.7 MIL LBS	SRI	MISC CHEMS	19.3 MIL LBS
DODECYLPHENOL, ETHOXYLATED		17.4 MIL LBS	T72	SURF-ACTIV AGENT	17.9 MIL LBS
N-HEXYL N-DECYL PHTHALATE		16.1 MIL LBS	T72	PLASTICIZERS	16.3 MIL LBS
MIXED LINEAR ALCOHOLS, ETHOXYLATED & SULFATED, SODIUM SALT		16.0 MIL LBS	SRI	SURF-ACTIV AGENT	16.5 MIL LBS
COCONUT OIL ACIDS, DIETHANOLAMINE CONDENSATE (AMINE/ACID=2/1)		15.4 MIL LBS	T72	SURF-ACTIV AGENT	15.8 MIL LBS
DODECYL MERCAPTANS		15.2 MIL LBS	T72	RUBBER-PROC CHEM	15.2 MIL LBS
N-(2,6-DIMETHYLMORPHOLINO)-2-BENZOTHIAZOLESULFENAMIDE	<	15.0 MIL LBS	SRI	RUBBER-PROC CHEM	
N-OXYDIETHYLENE-2-BENZOTHIAZOLESULFENAMIDE	<	15.0 MIL LBS	SRI	RUBBER-PROC CHEM	
N-TERT-BUTYL-2-BENZOTHIAZOLESULFENAMIDE	<	15.0 MIL LBS	SRI	RUBBER-PROC CHEM	
SILICONE RESINS (THERMOSETTING)		13.4 MIL LBS	T72	PLASTIC & RESIN	12.5 MIL LBS
GLYCEROL MONOESTER OF HYDROGENATED SOYBEAN OIL ACIDS		13.1 MIL LBS	T72	SURF-ACTIV AGENT	13.5 MIL LBS
STYRENE-ALKYD POLYESTERS		12.5 MIL LBS	T72	PLASTIC & RESIN	
OLEIC ACID, SULFATED, DISODIUM SALT		12.2 MIL LBS	T72	SURF-ACTIV AGENT	12.6 MIL LBS
GLYCEROL MONOESTER OF COCONUT OIL ACIDS		12.0 MIL LBS	SRI	SURF-ACTIV AGENT	12.4 MIL LBS
DODECYLDIPHENYLOXIDE DISULFONIC ACID, DISODIUM SALT		12.0 MIL LBS	SRI	SURF-ACTIV AGENT	12.4 MIL LBS
BIS(HYDROGENATED TALLOW ALKYL)AMINE		12.0 MIL LBS	SRI	SURF-ACTIV AGENT	12.4 MIL LBS
COCONUT OIL ACIDS, POTASSIUM SALT		11.9 MIL LBS	T72	SURF-ACTIV AGENT	
LEAD NAPHTHENATE		11.4 MIL LBS	T72	MISC CHEMS	
BUTYL OCTYL PHTHALATES		11.4 MIL LBS	T72	PLASTICIZERS	
BUTYL OCTYL PHTHALATES		11.4 MIL LBS	T72	PLASTICIZERS	
TALL OIL ACIDS, SODIUM SALT		10.7 MIL LBS	T72	SURF-ACTIV AGENT	
LAURIC ACID, DIETHANOLAMINE CONDENSATE (AMINE/ACID RATIO=1/1)		10.3 MIL LBS	SPI	SURF-ACTIV AGENT	
POLYACRYLONITRILE, HYDROLYZED		10.0 MIL LBS	SRI	PESTICIDES	
HEXADECYL SULFATE, SODIUM SALT		10.0 MIL LBS	SRI	SURF-ACTIV AGENT	
LIGNINSULFONIC ACID, ALUMINUM SALT		10.0 MIL LBS	SRI	SURF-ACTIV AGENT	
LIGNINSULFONIC ACID, IRON SALT		10.0 MIL LBS	SRI	SURF-ACTIV AGENT	
LIGNINSULFONIC ACID, MAGNESIUM SALT		10.0 MIL LBS	SRI	SURF-ACTIV AGENT	

Table 3-2 (continued)

OLIVE OIL ACIDS, SODIUM SALT	10.0 MIL LBS	SRI	SURF-ACTIV AGENT
ROSIN ACIDS, SODIUM SALT	10.0 MIL LBS	SRI	SURF-ACTIV AGENT
ALKYL PHENOL-FORMALDEHYDE CONDENSATES, ALKOXYLATED	9.4 MIL LBS	T72	SURF-ACTIV AGENT
DODECYL ALCOHOL, ETHOXYLATED	9.2 MIL LBS	T72	SURF-ACTIV AGENT
DODECYL ALCOHOL, ETHOXYLATED AND SULFATED, SODIUM SALT	9.0 MIL LBS	T72	SURF-ACTIV AGENT
ISO-OCTYL MERCAPTOACETATE	8.5 MIL LBS	T72	MISC CHEMS
CASTOR OIL, SULFATED, SODIUM SALT	8.3 MIL LBS	T72	SURF-ACTIV AGENT
ANHYDROSORBITOL MONOSTEARATE	8.0 MIL LBS	T72	SURF-ACTIV AGENT
(MIXED ALKYL)PHENOXYPOLY(ETHYLENEOXY)ETHYL CHLORIDE	8.0 MIL LBS	SRI	SURF-ACTIV AGENT
GLYCEROL MONOESTER OF TALLOW ACIDS	8.0 MIL LBS	SRI	SURF-ACTIV AGENT
GLYCEROL MONOESTER OF HYDROGENATED TALLOW ACIDS	8.0 MIL LBS	SRI	SURF-ACTIV AGENT
STEARYL & OTHER OCTADECYL ALCOHOLS	8.0 MIL LBS	T72	MISC CHEMS
NONYLPHENOL, ETHOXYLATED & PHOSPHATED	7.4 MIL LBS	T72	SURF-ACTIV AGENT
ETHOXYLATED ANHYDROSORBITOL MONO-OLEATE	7.0 MIL LBS	T72	SURF-ACTIV AGENT
PICOLINES, TOTAL	6.4 MIL LBS	T72	CYCLIC INTERMED
BENZYLDIMETHYL(MIXED ALKYL)AMMONIUM CHLORIDE	6.1 MIL LBS	T72	SURF-ACTIV AGENT
ISO-OCTYLPHENOL, ETHOXYLATED & SULFONATED, SODIUM SALT	6.0 MIL LBS	SRI	SURF-ACTIV AGENT
TRIDECYL ALCOHOL, ETHOXYLATED & SULFATED, SODIUM SALT	6.0 MIL LBS	SRI	SURF-ACTIV AGENT
M-(1-ETHYLPROPYL) & M-(1-METHYLBUTYL) PHENYL METHYLCARBAMATE	6.0 MIL LBS	SRI	PESTICIDES
TRIDECYL ALCOHOL, ETHOXYLATED & SULFATED, SODIUM SALT	6.0 MIL LBS	SRI	SURF-ACTIV AGENT
ANHYDROSORBITOL MONOLAURATE	5.9 MIL LBS	T72	SURF-ACTIV AGENT
PENICILLINS	5.9 MIL LBS	SRI	MEDICINAL CHEMS
CASTOR OIL, ETHOXYLATED	5.7 MIL LBS	T72	SURF-ACTIV AGENT
ETHOXYLATED ANHYDROSORBITOL MONOSTEARATE	5.4 MIL LBS	T72	SURF-ACTIV AGENT
(TALLOW ALKYL)AMINE	5.2 MIL LBS	T72	SURF-ACTIV AGENT
ROSIN ACIDS, POTASSIUM SALT	5.0 MIL LBS	SRI	SURF-ACTIV AGENT
COCONUT OIL ACIDS, 2-SULFOETHYL ESTER, SODIUM SALT	5.0 MIL LBS	SRI	SURF-ACTIV AGENT
9-OCTADECENYLAMINE	4.9 MIL LBS	T72	SURF-ACTIV AGENT
3,3'-DICHLOROBENZIDINE BASE AND SALTS	4.6 MIL LBS	T72	CYCLIC INTERMED
(N-HYDROXYETHYLENEDINITRILO)TRIACETIC ACID, TRISODIUM SALT	4.6 MIL LBS	T72	MISC CHEMS
TRIDECYL ALCOHOL, ETHOXYLATED	4.5 MIL LBS	T72	SURF-ACTIV AGENT
FURFURYL TYPE RESINS	4.5 MIL LBS	T72	PLASTIC & RESIN
(COCONUT OIL ALKYL)AMINE, ETHOXYLATED	4.4 MIL LBS	T72	SURF-ACTIV AGENT
MIXED FISH OILS, SULFATED, SODIUM SALT	4.3 MIL LBS	T72	SURF-ACTIV AGENT
ALKYLPHENOLS, ETHOXYLATED AND SULFATED	4.2 MIL LBS	T72	SURF-ACTIV AGENT
GLYCEROL MONOESTER OF HYDROGENATED COTTONSEED OIL ACIDS	4.2 MIL LBS	T72	SURF-ACTIV AGENT
TRIISO-OCTYL TRIMELLITATE	4.2 MIL LBS	T72	PLASTICIZERS
POLYIMIDE-TYPE RESINS	4.0 MIL LBS	SRI	PLASTIC & RESIN
MIXED LINEAR ALPHA OLEFINS, SULFONATED	4.0 MIL LBS	SRI	SURF-ACTIV AGENT
N-(TALLOW ALKYL)TRIMETHYLENEDIAMINE	4.0 MIL LBS	SRI	SURF-ACTIV AGENT
TETRACYCLINES	3.9 MIL LBS	T72	MEDICINAL CHEMS
(HYDROGENATED TALLOW ALKYL)AMINE	3.8 MIL LBS	T72	SURF-ACTIV AGENT
HYDROGENATED CASTOR OIL, ETHOXYLATED	3.7 MIL LBS	T72	SURF-ACTIV AGENT
CUMENESULFONIC ACID, AMMONIUM SALT	3.7 MIL LBS	T72	SURF-ACTIV AGENT
HYDROGENATED CASTOR OIL, ETHOXYLATED	3.7 MIL LBS	T72	SURF-ACTIV AGENT
MIXED LINEAR ALCOHOLS, ETHOXYLATED AND PHOSPHATED	3.6 MIL LBS	T72	SURF-ACTIV AGENT
OCTYLDIPHENYLAMINE	3.6 MIL LBS	T72	RUBBER-PROC CHEM
(DIETHYLENETRINITRILO)PENTAACETIC ACID, POTASSIUM SALT	3.5 MIL LBS	T72	MISC CHEMS
COBALT NAPHTHENATE	3.3 MIL LBS	T72	MISC CHEMS
SALICYLATES (EXCEPT ASPIRIN)	3.3 MIL LBS	T72	MEDICINAL CHEMS
BIS(COCONUT OIL ALKYL)DIMETHYLAMMONIUM CHLORIDE	3.3 MIL LBS	T72	SURF-ACTIV AGENT
NEAT'S-FOOT OIL, SULFATED, SODIUM SALT	3.2 MIL LBS	T72	SURF-ACTIV AGENT
(ETHYLENEDINITRILO)TETRAACETIC ACID, DI-NA ZN SALT, DIHYDRATE	3.1 MIL LBS	T72	MISC CHEMS
TRIOCTYL TRIMELLITATE	3.0 MIL LBS	T72	PLASTICIZERS
(SOYBEAN OIL ALKYL)AMINE	3.0 MIL LBS	SRI	SURF-ACTIV AGENT
(TALL OIL ALKYL)AMINE	3.0 MIL LBS	SRI	SURF-ACTIV AGENT
(COCONUT OIL ALKYL)AMINE	3.0 MIL LBS	SRI	SURF-ACTIV AGENT
GLYCEROL MONOESTER OF MIXED FATTY ACIDS, ACETYLATED	3.0 MIL LBS	SRI	SURF-ACTIV AGENT
ALKYLPHENOL, ETHOXYLATED	3.0 MIL LBS	SRI	SURF-ACTIV AGENT
(MIXED ALKYL)PHENOL-FORMALDEHYDE, ALKOXYLATED	3.0 MIL LBS	SRI	SURF-ACTIV AGENT
NONYLPHENOL-FORMALDEHYDE, ALKOXYLATED	3.0 MIL LBS	SRI	SURF-ACTIV AGENT

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Table 3-2 (continued)

GLYCEROL MONOESTER OF TALL OIL ACIDS	3.0	MIL LBS	SRI	SURF-ACTIV AGENT
COCONUT OIL & TALLOW ACIDS	3.0	MIL LBS	T72	SURF-ACTIV AGENT
MIXED LINEAR ALCOHOL SULFATE, TRIETHANOLAMINE SALT	3.0	MIL LBS	SRI	SURF-ACTIV AGENT
(MIXED ALKYL)AMINE, ETHOXYLATED	3.0	MIL LBS	SRI	SURF-ACTIV AGENT
TERPINEALS	3.0	MIL LBS	T72	FLAVOR & PERFUME
9-OCTADECENYL ALCOHOL, ETHOXYLATED	2.9	MIL LBS	T72	SURF-ACTIV AGENT
GLYCEROL MONO-OLEATE	2.8	MIL LBS	SRI	SURF-ACTIV AGENT
MIXED VEGETABLE FATTY ACIDS, POTASSIUM SALT	2.8	MIL LBS	T72	SURF-ACTIV AGENT
DODECYL ALCOHOL, ETHOXYLATED AND SULFATED, AMMONIUM SALT	2.7	MIL LBS	T72	SURF-ACTIV AGENT
MIXED LINEAR ALCOHOL SULFATE, SODIUM SALT	2.6	MIL LBS	SRI	SURF-ACTIV AGENT
ETHOXYLATED ANHYDROSORBITOL TRISTEARATE	2.5	MIL LBS	T72	SURF-ACTIV AGENT
TRIETHYLENE GLYCOL DI(CAPRYLATE-CAPRATE)	2.3	MIL LBS	T72	PLASTICIZERS
(TALLOW ALKYL)AMINE, ETHOXYLATED	2.2	MIL LBS	T72	SURF-ACTIV AGENT
N-METHYLBIS(HYDROGENATED TALLOW ALKYL)AMINE	2.2	MIL LBS	SRI	SURF-ACTIV AGENT
(TALLOW ALKYL)AMINE, ETHOXYLATED	2.2	MIL LBS	T72	SURF-ACTIV AGENT
TRI-N-OCTYL N-DECYL TRIMELLITATE	2.2	MIL LBS	T72	PLASTICIZERS
TRIMETHYLNONYL ALCOHOL, ETHOXYLATED	2.2	MIL LBS	T72	SURF-ACTIV AGENT
N-METHYLBIS(HYDROGENATED TALLOW ALKYL)AMINE	2.2	MIL LBS	T72	SURF-ACTIV AGENT
DICYANDIAMIDE RESINS	2.1	MIL LBS	T72	PLASTIC & RESIN
MIXED SUBSTITUTED OXIMES	2.0	MIL LBS	SRI	SURF-ACTIV AGENT
LEAD TALLATE	2.0	MIL LBS	T72	MISC CHEMS
ANHYDROSORBITOL MONOPALMITATE	2.0	MIL LBS	T72	SURF-ACTIV AGENT
TRIDECYLBENZENESULFONIC ACID	2.0	MIL LBS	SRI	SURF-ACTIV AGENT
N-(TALLOW ALKYL)TRIMETHYLENEDIAMINE, ETHOXYLATED	2.0	MIL LBS	SRI	SURF-ACTIV AGENT
(TALLOW ALKYL)AMINE ACETATE	2.0	MIL LBS	SRI	SURF-ACTIV AGENT
DODECYL SULFOACETATE, SODIUM SALT	2.0	MIL LBS	SRI	SURF-ACTIV AGENT
COD OIL, SULFATED, SODIUM SALT	2.0	MIL LBS	T72	SURF-ACTIV AGENT
N,N,N',N'-TETRAKIS(2-HYDROXYPROPYL)ETHYLENEDIAMINE, ALKOXYLATED	2.0	MIL LBS	SRI	SURF-ACTIV AGENT
LACTIC ACID SALTS	1.9	MIL LBS	T72	MISC CHEMS
N,N-DIMETHYL(COCONUT OIL ALKYL)AMINE	1.8	MIL LBS	SRI	SURF-ACTIV AGENT
PROPYL OLEATES (INCLUDING N-PROPYL OLEATE & ISOPROPYL OLEATE)	1.7	MIL LBS	T72	PLASTICIZERS
ISO-OCTYLPHENOL, ETHOXYLATED & SULFATED, SODIUM SALT	1.5	MIL LBS	SRI	SURF-ACTIV AGENT
BUTYL OLEATE, SULFATED, SODIUM SALT	1.5	MIL LBS	T72	SURF-ACTIV AGENT
N-(SOYBEAN OIL ALKYL)TRIMETHYLENEDIAMINE	1.5	MIL LBS	SRI	SURF-ACTIV AGENT
1-(2-AMINOETHYL)-2-NOR(TALL OIL ALKYL)-2-IMIDAZOLINE	1.5	MIL LBS	SRI	SURF-ACTIV AGENT
NONYLPHENOL, ETHOXYLATED AND SULFATED, AMMONIUM SALT	1.5	MIL LBS	SRI	SURF-ACTIV AGENT
OCTYLPHENOL, ETHOXYLATED AND SULFATED, SODIUM SALT	1.5	MIL LBS	SRI	SURF-ACTIV AGENT
SULFOSUCCINIC ACID DERIVATIVES	1.5	MIL LBS	T72	SURF-ACTIV AGENT
TRIDECYL ALCOHOL, ETHOXYLATED & PHOSPHATED	1.4	MIL LBS	T 72	SURF-ACTIV AGENT
COBALT TALLATE	1.3	MIL LBS	T72	MISC CHEMS
DECYL ALCOHOL, ETHOXYLATED	1.3	MIL LBS	T72	SURF-ACTIV AGENT
OCTADECYL ALCOHOL, ETHOXYLATED	1.3	MIL LBS	T72	SURF-ACTIV AGENT
OLEIC ACID SALTS	1.3	MIL LBS	T72	MISC CHEMS
HEXADECYL ALCOHOL, ETHOXYLATED	1.2	MIL LBS	T72	SURF-ACTIV AGENT
ALUMINUM MONOSTEARATE & TRISTEARATE	1.2	MIL LBS	T72	MISC CHEMS
MERCAPTOACETIC(THIOGLYCOLIC) ACID, SALTS	1.1	MIL LBS	T72	MISC CHEMS
DIRECT YELLOW 44	1.1	MIL LBS	T72	DYES
COCONUT OIL, SULFATED, SODIUM SALT	1.0	MIL LBS	T72	SURF-ACTIV AGENT
N,N-BIS(2-HYDROXYETHYL)(TALLOW ALKYL)AMINE	1.0	MIL LBS	SRI	SURF-ACTIV AGENT
(9-OCTADECENYL)AMINE, ETHOXYLATED	1.0	MIL LBS	SRI	SURF-ACTIV AGENT
GLYCEROL MONOSTEARATE, SUCCINYLATED	1.0	MIL LBS	SRI	SURF-ACTIV AGENT
BACILLUS THURINGIENSIS	1.0	MIL LBS	SRI	PESTICIDES
SULFOSUCCINIC ACID, DITRIDECYL ESTER, SODIUM SALT	1.0	MIL LBS	SRI	SURF-ACTIV AGENT
PETROLEUMSULFONIC ACID, WATER SOLUBLE (ACID LAYER), NA SALT	1.0	MIL LBS	SRI	SURF-ACTIV AGENT
XYLENESULFONIC ACID, POTASSIUM SALT	1.0	MIL LBS	SRI	SURF-ACTIV AGENT
SULFOSUCCINIC ACID, DIHEXYL ESTER, SODIUM SALT	1.0	MIL LBS	SRI	SURF-ACTIV AGENT
BIS(COCONUT OIL ALKYL)AMINE	1.0	MIL LBS	SRI	SURF-ACTIV AGENT
TALL OIL ACIDS, ETHANOLAMINE CONDENSATE (AMINE/ACID RATIO=[illegible])	1.0	MIL LBS	SRI	SURF-ACTIV AGENT

B. Identification of NSF Chemicals in EMIC Files

Using the CAS numbers as a means of comparison, the 436 CAS-numbered chemicals from the NSF study (shown in Table 3-1) were then compared with the 5162 chemicals with CAS numbers in the file of the Environmental Mutagen Information Center (EMIC). This is a computerized bibliographic file of worldwide literature on environmental mutagenesis and closely related studies such as the effects of chemicals on DNA synthesis, mitotic index, and synthetic polynucleotides. A table of the resulting 181 chemicals was then generated (Table 3-3). In this table, the first line beginning with an N contains the economic information on the CAS-numbered chemicals as described in Section III.A above. Each N line following the first contains CAS number, a synonym, and an acronym for the source reference of that name. If the synonym is blank or an "MX" code, the source reference acronym means that information about the chemical is to be found in that source. These synonyms were obtained from SRI's tape of 26,000 commercially significant chemicals produced as part of a project for the NCI. An explanation of the acronyms and the associated references is given in Table 3-4. The first line beginning with an E contains the CAS number and the number of E lines which follow. Subsequent E lines contain the number (1-18) of EMIC accession numbers (corresponding to literature references) on that line followed by those accession numbers.

Table 3-3. NSF CHEMICALS IN EMIC FILES

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N 000050000  FORMALDEHYDE (37% BY WEIGHT)                                     5651.8 MIL LBS  T72  MISC CHEMS           52.3 MIL LB
N 000050000 FORMALDEHYDE                                                          FC
N 000050000 FORMALCEHYDE                                                          DC
N 000050000 FCRMALCFHYDE                                                          NP
N 000050000                                                                      CEH
N 000050000 MX8049352                                                             MX
N 000050000 MX8005387                                                             MX
N 000050000 FORMALDEHYDE                                               158163 169100
N 000050000 MX8006073                                                             MX
N 000050000 MX8013136                                                             MX
N 000050000 FORMALDEHYDE                                                          FA
N 000050000 FORMALCEHYDE                                                           P
N 000050000 FORMALDEHYDE                                                          PD
N 000050000 FORMALCEHYDE                                                          FA
N 000050000 MX8053847                                                             MX
N 000050000 MX8022911                                                             MX
N 000050000 MX8047469                                                             MX
N 000050000 FORMALDEHYDE                                                      161JSO
N 000050000 FORMALDEHYCE                                                          CT
N 000050000 ANTIBACTERIAL AGENT %E.G. FORMALDEHYDE<                               CT
N 000050000 FORMALDEHYDE                                                          CT
N 000050000 FORMALIN (FORMALDEHYDE)                                                C
N 000050000 FORMALDEHYCE                                                          FR
N 000050000
E 000050000 0007
E 18 004504 004592 004597 004616 004673 004689 004697 004869 004883 004918 005009 005146 005180 005181 005255 005412 005512 005685
E 18 005693 006332 006727 006783 006827 006853 006905 006911 006912 006917 007092 007100 007342 007589 007908 007962 008077 008360
E 18 008584 008715 009437 009481 009482 009487 009488 009526 009561 010150 010424 010506 010523 010536 010539 010579 010600 010617
E 18 010618 010621 010687 010742 010759 010799 010817 010843 010937 010938 010965 011001 011016 011067 011144 011162 011322 011325
E 18 011329 011468 011504 011605 011962 012304 012479 012484 012826 012979 012984 013350 013373 013440 013451 013733 014031 014346
E 18 014851 014852 014886 015385 015406 015548 015688 015773 016079 016585 016765 017167 017193 017386 018293 018456 018746 019227
E 15 019324 019839 020007 020387 020777 020819 020899 021260 021355 021718 021804 021955 022382 022411 022807

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N 000050293  DDT                                                                45.0 MIL LBS  SRI  PESTICIDES           41.5 MIL LB
N 000050293 MX8017343                                                             MX
N 000050293                                                                      CEH
N 000050293 1,1,1-TRICHLORO-2,2-BIS(P-CHLOROPHENYL)ETHANE              240296 292313
N 000050293 MX8003029                                                             MX
N 000050293
N 000050293 MX805612C                                                             MX
N 000050293 1,1,1-TRICHLORO-2,2-BIS(P-CHLOROPHENYL)ETHANE                      10DSC
N 000050293 DDT                                                                   CT
N 000050293 DICHLORODIPHENYL TRICHLORCETHANE                                      CT
E 000050293 0005
E 18 004625 004647 004888 005896 005995 006453 006589 007234 007252 007618 008197 008204 008211 008893 009043 009124 009468 009588
E 18 010171 010636 010737 010806 010851 011061 011141 011347 011509 012383 012485 012578 012821 012984 012999 013135 013248 013330
E 18 013528 013595 013608 014027 014070 014098 014101 014190 014440 014446 014686 014687 014813 014967 015428 016741 016828 018335
E 18 018480 018707 018783 019564 020036 020178 020315 020756 020762 020941 021234 021300 021385 021572 021606 022342 022345 022818
E 01 022827

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N 000050704  SORBITOL                                                          121.4 MIL LBS  T72  MISC CHEMS           52.2 MIL LB
N 000050704 D-GLUCITOL                                                        599CSO
N 000050704 SORBITCL                                                              FA
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Table 3-3 (continued)

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N 000050704 MX8048268                                                MX
N 000050704 MX8058295                                                MX
N 000050704 SORBITOL                                                 CT
N 000050704 HUMECTANTS %E.G. SORBITOL<                               CT
N 000050704 POLYOLS %E.G. SORBITOL<                                  CT
N 000050704 SORBITOL                                                 CT
N 000050704 SORBITOL                                                 CT
N 000050704 D-SORBITOL                                               CT
N 000050704                                                          CEH
N 000050704 SUSP SORBITOL %SORBITOL<                                 NP
N 000050704 SORBITOL                                                 DC
N 000050704 SORBITOL                                                 NP
N 000050704 SORBITOL                                                 FC
N 000050704 SORBITOL                                                 FC
N 000050704 SORBITOL                                                 FC
N 000050704 SORBITOL                                                 FC
N 000050704 MX8013158                                                MX
N 000050704
E 000050704 0001
E 04 006556 011876 017280 020877

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N 000050782  ASPIRIN                                                35.0 MIL LBS  T72  MEDICINAL CHEMS      35.9 MIL LB
N 000050782                                                         CEH
N 000050782 MX8013169                                                MX
N 000050782 ASPIRIN                                                  NP
N 000050782
N 000050782 MX8055376                                                MX
N 000050782 MX8054726                                                MX
N 000050782 MX8056200                                                MX
N 000050782 MX8056211                                                MX
N 000050782 MX8056233                                                MX
N 000050782 MX8056222                                                MX
N 000050782 MX8056131                                                MX
N 000050782 MX8054679                                                MX
N 000050782 ASPIRIN                                                  PD
N 000050782 ASPIRIN                                                  HA
N 000050782 ACETYLSALICYLIC ACID                                 038DSO
N 000050782 MX8058308                                                MX
N 000050782 MX8058331                                                MX
N 000050782 MX8058320                                                MX
N 000050782 MX8057918                                                MX
N 000050782 MX8058353                                                MX
N 000050782 MX8058319                                                MX
N 000050782 MX8058342                                                MX
N 000050782 ACETYLSALICYLIC ACID                                     DC
N 000050782 ASPIRIN                                                  CD
E 000050782 0002
E 18 005300 005337 006175 009113 009114 009115 009468 011585 011600 011731 016542 018635 019793 020147 020278 021412 021434 021451
E 01 021463

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N 000050817  VITAMIN C
N 000050817 ASCORBIC ACID (C)                                       15.6 MIL LBS  T72  MEDICINAL CHEMS      21.1 MIL LB
N 000050817 ASCORBIC ACID                                            CD
                                                                     DC
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Table 3-3 (continued)

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N 000050817
N 000050817 MX8058397                                                           MX
N 000050817 MX8058024                                                           MX
N 000050817 MX8058386                                                           MX
N 000050817 MX8058375                                                           MX
N 000050817 MX8058400                                                           MX
N 000050817 MX8058308                                                           MX
N 000050817 MX8026311                                                           MX
N 000050817 MX8058411                                                           MX
N 000050817 MX8058364                                                           MX
N 000050817 ASCORBIC ACID                                                       HA
N 000050817 ASCORBIC ACIC                                                       PD
N 000050817 MX8056244                                                           MX
N 000050817 MX8056095                                                           MX
N 000050817 MX8055387                                                           MX
N 000050817 MX8054737                                                           MX
N 000050817 MX8054748                                                           MX
N 000050817 MX8056266                                                           MX
N 000050817 MX8053881                                                           MX
N 000050817 MX8054726                                                           MX
N 000050817 MX8053507                                                           MX
N 000050817 MX8056288                                                           MX
N 000050817 MX8053712                                                           MX
N 000050817 MX8056255                                                           MX
N 000050817 MX8056277                                                           MX
N 000050817 ASCORBIC ACID                                                   596CSO
N 000050817 MX8061834                                                           MX
N 000050817 MX8061572                                                           MX
N 000050817 MX8061685                                                           MX
N 000050817 MX8061130                                                           MX
N 000050817 ASCORBIC ACIC                                                       FA
N 000050817 ASCORBIC ACID                                                       NP
N 000050817 VITAMIN C                                                           NP
N 000050817 MX8026322                                                           MX
N 000050817 MX8026344                                                           MX
N 000050817 MX8028044                                                           MX
N 000050817 MX8026333                                                           MX
N 000050817 MX8026355                                                           MX
N 000050817                                                                    CEH
N 000050817 MX8046955                                                           MX
N 000050817 L-ASCORBIC ACID                                        1169761    598
N 000050817 ASCORBIC ACID (VITAMIN C)                                           FC
N 000050817 ASCORBIC ACID (VITAMIN C)                                           FC
N 000050817 MX8012224                                                           MX
N 000050817 MX8048928                                                           MX
E 000050817 0002
E 18 004614 008648 009270 010244 010757 010902 011059 011162 011298 012503 012643 012978 014038 014375 016572 016941 017524 017804
E 10 017849 018397 018922 019650 019795 020741 021421 021697 022326 022355

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N 000051036  PIPERONYL BUTOXIDE                                                1.0 MIL LBS   SRI  PESTICIDES
N 000051036 MX8026366                                                           MX
N 000051036 MX8046795                                                           MX
N 000051036                                                                    CEH
N 000051036 A-(2-(2-BUTOXYMETHOXY)ETHCXY)-4,5-METHYLENEDIOXY-2-PRCP    906 923616
N 0000510361YLTOLUENE
N 000051036 ALPHA-(2-(2-BUTOXYETHOXY)ETHOXY)-4,5-(METHYLENECICXY)-2-PROPYLTO489GSO
N 0000510361LUENE                                                           489GSO
```

Table 3-3 (continued)

```
N 000051036 PIPEFCNYL BUTOXIDE                                                   CT
N 000051036
N 000051036 MX8063691                                                            MX
N 000051036 MX8C63692                                                            MX
N 000051036 PIPERONYL BUTOXIDE-TECHNICAL                                          P
N 000051036 PIPERCNYL BUTCXIDE                                                    P
E 000051036 0001
E 03 012984 014190 022326

---------------------------------------------------------------------------------------------------------------------------------

N 000056235  CARBON TETRACHLCRIDE                                             996.7 MIL LBS  T72  MISC CHEMS          105.0 MIL LB
N 000056235 MX8058784                                                            MX
N 000056235                                                                     CEH
N 000056235 MX8058773                                                            MX
N 000056235 MX8003063                                                            MX
N 000056235 MX8003074                                                            MX
N 000056235 MX8002811                                                            MX
N 000056235 CARBON TETRACHLCRIDE                                       119107 124 62
N 000056235 CARBON TETRACHLORIDE                                                 DC
N 000056235 MX8063705                                                            MX
N 000056235 CARBON TETRACHLORIDE                                              12CSO
N 000056235 CARBON TETRACHLORIDE                                                 CT
N 000056235
E 000056235 0002
E 18 004413 004442 004485 008531 008705 008827 010803 012083 012961 013509 014069 014382 015985 016439 017328 018910 020156 020308
E 05 020562 021337 021557 021958 021994

---------------------------------------------------------------------------------------------------------------------------------

N 000056382  PARATHICN                                                         15.0 MIL LBS  SRI  PESTICIDES           15.2 MIL LB
N 000056382                                                                     CEH
N 000056382 MX8003983                                                            MX
N 000056382
N 000056382 ETHYL PARATHION                                                       P
N 000056382 PARATHION (ETHYL PARATHION)                                           P
N 000056382 PHOSPHOROTHIOIC ACID,O,O-DIETHYL C,P-NITROPHENYL ESTER            35CSC
E 000056382 0001
E 16 004498 005126 009468 010464 012603 013784 014717 016163 016302 016741 018997 019358 020762 021918 022877 022878

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N 000056815  GLYCEROL, SYNTHETIC ONLY                                         199.2 MIL LBS  T72  MISC CHEMS           89.4 MIL LB
N 000056815 GLYCERIN                                                             PD
N 000056815 GLYCEROL                                                             FA
N 000056815 MX8053063                                                            MX
N 000056815 MX805484C                                                            MX
N 000056815 MX8050995                                                            MX
N 000056815 MX8056448                                                            MX
N 000056815 MX8054851                                                            MX
N 000056815 MX8052617                                                            MX
N 000056815 MX8054839                                                            MX
N 000056815 MX8050962                                                            MX
N 000056815 MX8022591                                                            MX
N 000056815 MX8048155                                                            MX
```

Table 3-3 (continued)

```
N 000056815 MX8047367                                                          MX
N 000056815 MX8024213                                                          MX
N 000056815 MX8047390                                                          MX
N 000056815 MX8058319                                                          MX
N 000056815 MX8047345                                                          MX
N 000056815 MX8047663                                                          MX
N 000056815 MX8048371                                                          MX
N 000056815 MX8047107                                                          MX
N 000056815 MX8048268                                                          MX
N 000056815 J08060502                                                          MX
N 000056815 MX8063567                                                          MX
N 000056815 MX8061970                                                          MX
N 000056815 GLYCEROL                                                       1638SC
N 000056815 MX8049432                                                          MX
N 000056815 MX8012280                                                          MX
N 000056815 MX8011425                                                          MX
N 000056815 MX8048984                                                          MX
N 000056815 MX8050688                                                          MX
N 000056815 MX8012291                                                          MX
N 000056815 MX8048882                                                          MX
N 000056815 MX8049363                                                          MX
N 000056815 MX8048973                                                          MX
N 000056815 MX8006095                                                          MX
N 000056815 MX8058842                                                          MX
N 000056815 MX8017081                                                          MX
N 000056815 MX8021816                                                          MX
N 000056815 MX8021827                                                          MX
N 000056815                                                                   CEH
N 000056815 MX8047027                                                          MX
N 000056815 GLYCERIN                                                           NP
N 000056815 ANHYDRCUS GLYCERIN                                                 NP
N 000056815 GLYCERINE                                                          DC
N 000056815 MX9028920                                                          MX
N 000056815 MX8027609                                                          MX
N 000056815 MX8013250                                                          MX
N 000056815 MX8030362                                                          MX
N 000056815 MX8013261                                                          MX
N 000056815 MX8026708                                                          MX
N 000056815 MX8030259                                                          MX
N 000056815 MX8028555                                                          MX
N 000056815 MX8029990                                                          MX
N 000056815 MX8028919                                                          MX
N 000056815 MX8030839                                                          MX
N 000056815 GLYCERIN (GLYCEROL)                                                FC
N 000056815 GLYCERIN CEHYDRATED                                                CD
N 000056815 GLYCEROL                                                           FR
N 000056815 GLYCERIN (GLYCERINE) (GLYCEROL)                                    CT
N 000056815 GLYCEROL                                                           CT
N 000056815 GLYCERCL                                                           CT
N 000056815 GLYCEROL                                                           CT
N 000056815
E 000056815 0001
E 15 004453 006125 008026 008102 009270 [illegible]432 [illegible]10593 012089 013209 013911 015242 016090 016494 019340 019834

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N 000057136  UREA                                                          13320.0 MIL LBS  SRI  MISC CHEMS      11622.1 MIL LB
N 000057136 UREA                                                               CT
N 000057136
```

Table 3-3 (continued)

```
N 000057136 MX8058853                                                             MX
N 000057136 MX8017503                                                             MX
N 000057136                                                                      CEH
N 000057136 MX8017514                                                             MX
N 000057136 UREA                                                                  DC
N 000057136 CARBAMIDE                                                             NP
N 000057136 UREA                                                                  NP
N 000057136 UREA                                                                  FC
N 000057136 MX8027610                                                             MX
N 000057136 MX8006108                                                             MX
N 000057136 MX8005398                                                             MX
N 000057136 MX8000122                                                             MX
N 000057136 UREA                                                                  HA
N 000057136 UREA                                                              195DSO
N 000057136 MX8048177                                                             MX
N 000057136 MX8023083                                                             MX
N 000057136 MX8023094                                                             MX
N 000057136 UREA                                                                  PD
N 000057136 MX8056460                                                             MX
N 000057136 MX8053983                                                             MX
N 000057136 MX8053996                                                             MX
E 000057136 0002
E 18 005066 005412 005771 006983 008026 008102 008512 008866 010439 010817 012089 012691 012979 014213 014965 015568 016233 016532
E 06 018566 019821 020784 020992 021600 022850

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N 000057556  PROPYLENE GLYCOL                                                  562.6 MIL LBS  T72  MISC CHEMS          154.0 MIL LB
N 000057556 1,2-PROPANEDIOL                                          183    229146
N 000057556 MX8000122                                                             MX
N 000057556 MX8046671                                                             MX
N 000057556                                                                      CEH
N 000057556 MX8017547                                                             MX
N 000057556 MX8012315                                                             MX
N 000057556 MX8048871                                                             MX
N 000057556 MX8030384                                                             MX
N 000057556 PROPYLENE GLYCOL                                                     KEP
N 000057556 MX8027610                                                             MX
N 000057556 MX8026479                                                             MX
N 000057556 MX8026480                                                             MX
N 000057556 MX8028566                                                             MX
N 000057556 PROPYLENE GLYCOL
N 000057556 PROPYLENE GLYCOL                                                      FC
N 000057556 MX8022615                                                             MX
N 000057556 MX8023118                                                             MX
N 000057556 MX8023583                                                             MX
N 000057556 MX8023083                                                             MX
N 000057556 MX8022604                                                             MX
N 000057556 MX8048144                                                             MX
N 000057556 MX8024213                                                             MX
N 000057556 MX8023027                                                             MX
N 000057556 MX8023094                                                             MX
N 000057556 MX8023129                                                             MX
N 000057556 MX8024202                                                             MX
N 000057556 MX8052297                                                             MX
N 000057556 MX8054011                                                             MX
N 000057556 1,2-PROPANEDIOL                                                   184ISO
N 000057556
E 000057556 0001
```

Table 3-3 (continued)

```
E 01 020895

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N 000057749  CHLCRDAN                                                         25.0 MIL LBS  SRI  PESTICIDES          25.3 MIL LB
N 000057749
N 000057749                                                                      CEH
N 0000577491N                                                                 176ISO
N 000057749 1,2,4,5,6,7,8,8-CCTACHLORC-3A,4,7,-7A-TETRAHYDRO-4,7-METHANOINDA176ISO
N 000057749 CHLORDANE (CCTACHLORO-4,7-METHANO-TETRAHYCROINDANE)                    P
N 000057749 CHLORDANE                                                             CT
N 000057749 OCTACHLORO-4,7 METHANOTETRAINDANE %CHLORDANE<                         CT
E 000057749 0001
E 10 005649 008197 009044 009060 009124 011141 012984 013248 013330 014190

-----------------------------------------------------------------------------------------------------------------

N 000059029  VITAMIN E                                                         2.9 MIL LBS  T72  MEDICINAL CHEMS
N 000059029 MX8048428                                                             MX
N 000059029 MX8026311                                                             MX
N 000059029 MX8026286                                                             MX
N 000059029 MX8056700                                                             MX
N 000059029 2,5,7,8-TETRAMETHYL-2-(4,8,12-TRIMETHYLTRIDECYL)-6-CHROMANOL    288DSO
N 000059029
N 000059029 MX8017309                                                             MX
N 000059029 MX8017296                                                             MX
N 000059029 MX8026640                                                             MX
N 000059029 VITAMIN E (WHEAT GERM OIL)                                            DC
N 000059029 VITAMIN E                                                             NP
N 000059029 2,5,7,8-TETRAMETHYL-2-(4,8,12-TRIMETHYLTRIDECYL)-6-CHR01309    973793
N 0000590291MANOL
E 000059029 0001
E 06 010902 011403 015578 018583 021603 022460

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N 000060297  ETHYL ETHER, TECHNICAL                                           69.4 MIL LBS  T72  MISC CHEMS          35.7 MIL LB
N 000060297                                                                      CEH
N 000060297 ETHER                                                                 NP
N 000060297 ETHYL ETHER                                                           DC
N 000060297 MX8013432                                                             MX
N 000060297 MX8013034                                                             MX
N 000060297 MX8013454                                                             MX
N 000060297 MX8013443                                                             MX
N 000060297 MX8050699                                                             MX
N 000060297 MX8011436                                                             MX
N 000060297 ETHYL ETHER                                                       264DSO
N 000060297 MX8056744                                                             MX
N 000060297 MX8055514                                                             MX
N 000060297 ETHYL ETHER                                                           AR
N 000060297 DIETHYL ETHER                                                         CT
N 000060297 ETHYL ETHER MEDICINAL                                          9439  CEH
N 000060297 ETHYL ETHER                                                           FR
N 000060297
E 000060297 0001
```

Table 3-3 (continued)

```
E 09 004630 004872 005695 006978 009335 010377 013425 019071 021321

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N 000060515  DIMETHOATE                                                        2.0 MIL LBS  SRI  PESTICIDES
N 000060515 DIMETHOATE (CYGON)                                                   P
N 000060515 DIMETHOATE                                                           P
N 000060515
N 000060515 PHOSPHORODITHIOIC ACID, O,O-DIMETHYL ESTER, S-ESTER WITH 2-MERCA315GSO
N 0000605151PTC-N-METHYLACETAMIDE                                           315GSO
N 000060515                                                                    CEH
E 000060515 0002
E 18 010953 014074 014190 014528 014808 016163 016302 016475 016741 017984 018326 018984 019775 020176 020762 021385 021856 021918
E 02 022418 022827

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N 000062533  ANILINE (ANILINE OIL)                                           409.8 MIL LBS  T72  CYCLIC INTERMED
N 000062533                                                                    CEH
N 000062533 ANILINE                                                         107ASO
N 000062533 ANILINE                                                             PR
N 000062533
N 000062533 ANILINE                                                             CT
N 000062533 AROMATIC AMINES %E.G. ANILINE<                                      CT
E 000062533 0001
E 06 004630 005695 010652 012660 017303 021337

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N 000063252  CARBARYL                                                       <  55.0 MIL LBS  SRI  PESTICIDES             50.5 MIL LB
N 000063252 CARBARYL                                                            P
N 000063252 SEVIN                                                               P
N 000063252 METHYLCARBAMIC ACID, 1-NAPHTHYL ESTER                           276GSO
N 000063252
N 000063252                                                                    CEH
N 000063252 METHYLCARBAMIC ACID, 1-NAPHTHYL ESTER                             335
N 000063252 MX8026366                                                           MX
N 000063252 CARBARYL                                                            CT
N 000063252 1-NAPHTHYL N-METHYLCARBAMATE                                        CT
E 000063252 0003
E 18 006546 009468 009537 009588 010771 010772 010779 010791 011281 012984 013248 013397 013445 013458 014190 014264 014472 014605
E 18 015340 016191 016741 016756 017079 017537 018005 018427 020762 021186 021337 021344 021385 021606 021759 021799 022308 022818
E 02 022827 022838

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N 000064028  (ETHYLENEDINITRILO)TETRAACETIC ACID, TETRASODIUM SALT            64.3 MIL LBS  T72  MISC CHEMS              65.3 MIL LB
  000064028 SODIUM EDTA                                                         CT
N 000064028 TETRASODIUM ETHYLENE DIAMINETETRA ACETATE (EDTA TETRASODIUM)         C
N 000064028                                                                    CEH
N 000064028 MX8059221                                                           MX
N 000064028 MX8013501                                                           MX
N 000064028 MX8013512                                                           MX
```

Table 3-3 (continued)

```
N 000064028 MX8013498                                                     MX
N J00064028 (ETHYLENEDINITRILO)TETRAACETIC ACID TETRASODIUM SALT       22FSO
N 000064028 TETRASODIUM ETHYLENEDIAMINETETRAACETATE                      FDA
N 000064028
E 000064028 0001
E 01 008026

------------------------------------------------------------------------------------------------------

N 000064175  ETHYL ALCCHOL, SYNTHETIC                                 1850.7 MIL LBS  T72  MISC CHEMS         581.7 MIL LB
N 000064175 ALCOHOL                                                       FA
N 000064175 ETHYL ALCOHOL                                             263BSO
N 000064175 ETHYL ALCCHCL (ETHANCL)                                       FA
N 000064175 SHERRY WINE (E.G.ETHANOL)                                     FA
N 000064175 BRANDY (ETHNOL)                                               FA
N 000064175 MX8060671                                                     MX
N 000064175 WINE (E.G. ETHANOL)                                           FA
N 000064175 ETHYL ALCOHOL                                                 AR
N 000064175 ETHYL ALCOHOL                                                 PR
N 000064175 MX8047312                                                     MX
N 000064175 MX8047243                                                     MX
N 000064175 MX8048462                                                     MX
N 000064175 MX8023118                                                     MX
N 000064175 MX8047947                                                     MX
N 000064175 MX8048144                                                     MX
N 000064175 MX8047196                                                     MX
N 000064175 MX8047174                                                     MX
N 000064175 MX8047936                                                     MX
N 000064175 MX8048199                                                     MX
N 000064175 MX8048155                                                     MX
N 000064175 MX8047209                                                     MX
N 000064175 MX8023232                                                     MX
N 000064175 ALCOHOL                                                       PD
N 000064175 MX8050995                                                     MX
N 000064175 MX8052253                                                     MX
N 000064175 MX8056857                                                     MX
N 000064175 MX8052173                                                     MX
N 000064175 MX8050962                                                     MX
N 000064175 MX8054146                                                     MX
N 000064175 MX8052220                                                     MX
N 000064175 MX8053165                                                     MX
N 000064175 MX8052322                                                     MX
N 000064175 MX8052775                                                     MX
N 000064175 MX8053994                                                     MX
N 000064175 MX8052219                                                     MX
N 000064175 MX8055058                                                     MX
N 000064175 ALCOHOL (ETHYL, GRAIN, DENATURED, ETC.)                       OC
N 000064175 ETHANOL                                                       CT
N 000064175 ETHANOL                                                       CT
N 000064175 ETHYL ALCOHOL                                                  C
N 000064175 ALCOHCL %E.G. C2H5OH<                                         CT
N 000064175 ETHYL ALCOHOL                                                 FR
N 000064175 ETHYL ALCOHCL                                                 FR
N 000064175 ALCOHOL                                                       CT
N 000064175 ALCOHOL (ETHANUL)                                             CD
N J00064175 MX8017763                                                     MX
N 000064175                                                              CEH
N 000064175 MX8021850                                                     MX
N 000064175 MX8059232                                                     MX
```

Table 3-3 (continued)

```
N 000064175 MX8017116                                                            MX
N 000064175 MX8047083                                                            MX
N 000064175 MX8013523                                                            MX
N 000064175 MX8013443                                                            MX
N 000064175 MX8013545                                                            MX
N 000064175 MX8026693                                                            MX
N 000064175 MX8013125                                                            MX
N 000064175 MX8046588                                                            MX
N 000064175 MX8013329                                                            MX
N 000064175 MX8028931                                                            MX
N 000064175 MX8013089                                                            MX
N 000064175 MX8026719                                                            MX
N 000064175 MX8027961                                                            MX
N 000064175 MX8046944                                                            MX
N 000064175 MX8030384                                                            MX
N 000064175 MX8013567                                                            MX
N 000064175 MX8030362                                                            MX
N 000064175 MX8030339                                                            MX
N 000064175 MX8030419                                                            MX
N 000064175 MX8030839                                                            MX
N 000064175 MX8030293                                                            MX
N 000064175 MX8013578                                                            MX
N 000064175 MX8028920                                                            MX
N 000064175 MX8013556                                                            MX
N 000064175 MX8047050                                                            MX
N 000064175 MX8013432                                                            MX
N 000064175 MX8012859                                                            MX
N 000064175 MX8047038                                                            MX
N 000064175 MX8030000                                                            MX
N 000064175 MX8013589                                                            MX
N 000064175 MX8047072                                                            MX
N 000064175 MX8030259                                                            MX
N 000064175 MX8013590                                                            MX
N 000064175 MX8027621                                                            MX
N 000064175 MX8028919                                                            MX
N 000064175 MX8047005                                                            MX
N 000064175 MX8013534                                                            MX
N 000064175 MX8013603                                                            MX
N 000064175 MX8028555                                                            MX
N 000064175 ETHYL ALCOHCL (ETHANOL)                                              FC
N 000064175 ALCOHOL                                                              NP
N 000064175 ETHYL ALCOHOL                                                        NP
N 000064175 MX8030166                                                            MX
N 000064175 ETHYL ALCOHOL                                           146149 156 92
N 000064175 MX8003154                                                            MX
N 000064175 MX8050699                                                            MX
N 000064175 MX8050439                                                            MX
N 000064175 MX8048871                                                            MX
N 000064175 MX8050393                                                            MX
N 000064175 MX8012360                                                            MX
N 000064175 MX8050359                                                            MX
N 000064175 MX8012371                                                            MX
N 000064175
E 000064175 0003
E 18 004492 004625 004630 004675 004690 004756 005254 005532 005586 005756 005961 005993 006717 006978 007004 007117 007618 007797
E 18 007971 008282 009493 010535 010766 010817 011445 011731 011819 012089 012169 012655 013740 013911 015366 016090 016216 016451
E 15 016496 016515 018650 019340 019923 020004 020031 020156 020291 020393 020674 021337 021400 022052 022850
```

Table 3-3 (continued)

```
N 000064186  FORMIC ACID                                         46.9 MIL LBS  T72  MISC CHEMS          24.1 MIL LB
N 000064186 MX8007441                                              MX
N 000064186 MX8011447                                              MX
N 000064186 MX8006937                                              MX
N 000064186 FORMIC ACID                                           101
N 000064186 MX8007043                                              MX
N 000064186 FORMIC ACID                                            DC
N 000064186 FORMIC ACID                                            SF
N 000064186                                                        CEH
N 000064186 FORMIC ACID                                            FC
N 000064186
N 000064186 MX8053847                                              MX
N 000064186 FORMIC ACID                                          162CSO
E 000064186 0001
E 06 004883 004951 006783 006911 006912 016079

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N 000064197  ACETIC ACID, SYNTHETIC, 100%                      2235.0 MIL LBS  T72  MISC CHEMS          55.9 MIL LB
N 000064197 ACETIC ACID                                        073CSO
N 000064197 MX8022739                                              MX
N 000064197 MX8024122                                              MX
N 000064197 MX8023243                                              MX
N 000064197 MX8022751                                              MX
N 000064197 MX8047947                                              MX
N 000064197 ETHANOIC ACID (ACETIC ACID)                            FA
N 000064197 ACETIC ACID                                            FA
N 000064197 ACETIC ACID                                            CT
N 000064197 ACETIC ACID                                            DC
N 000064197 ACETIC ACID                                            FC
N 000064197                                                        CEH
N 000064197 ACETIC ACID                                            FC
N 000064197 ACETIC ACID                                            SF
N 000064197 ACETIC ACID                                            NP
N 000064197 GLACIAL ACETIC ACID                                    NP
N 000064197 MX8007043                                              MX
N 000064197 MX8006926                                              MX
N 000064197 MX8006131                                              MX
N 000064197 ACETIC ACID                               106 90      36
N 000064197 MX8049498                                              MX
N 000064197 MX8007441                                              MX
N 000064197 MX8012382                                              MX
N 000064197 MX8013614                                              MX
N 000064197 MX8013307                                              MX
N 000064197
E 000064197 0001
E 12 004883 006783 006911 006912 008904 011258 011278 01299[illegible] 014032 014387 018942 021337

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N 000065850  BENZOIC ACID, TECH.                                  155.5 MIL LBS  T72  CYCLIC INTERMED
N 000065850 BENZOIC ACID                                           DC
N 000065850 BENZOIC ACID                                           CT
N 000065850 BENZOIC ACID                                           FC
N 000065850 BENZOIC ACID                                           SF
N 000065850 BENZOIC ACID                                           FC
```

Table 3-3 (continued)

```
N 000065850                                                                      CEH
N 000065850 BENZOIC ACID                                                          NP
N 000065850 MX8013636                                                             MX
N 000065850 MX8038651                                                             MX
N 000065850 MX8029990                                                             MX
N 000065850 MX8011890                                                             MX
N 000065850 MX8050688                                                             MX
N 000065850 MX8007805                                                             MX
N 000065850
N 000065850 MX8047210                                                             MX
N 000065850 MX8047232                                                             MX
N 000065850 MX8024235                                                             MX
N 000065850 MX8047345                                                             MX
N 000065850 MX8047390                                                             MX
N 000065850 MX8047389                                                             MX
N 000065850 MX8023947                                                             MX
N 000065850 MX8023607                                                             MX
N 000065850 MX8047221                                                             MX
N 000065850 MX8053165                                                             MX
N 000065850 MX8061970                                                             MX
N 000065850 BENZOIC ACID                                                      071ESO
N 000065850 BENZOIC ACID                                                          FA
E 000065850 0001
E 05 009270 010648 020784 021337 021384

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N 000067481  CHOLINE CHLORIDE (ALL GRADES)                                      54.5 MIL LBS  T72  MEDICINAL CHEMS       56.1 MIL LB
N 000067481
N 000067481                                                                      CEH
N 000067481 MX8059298                                                             MX
N 000067481 MX8050519                                                             MX
N 000067481 CHOLINE CHLORIDE                                                      FC
N 000067481 CHOLINE CHLORIDE                                                      FA
N 000067481 CHOLINE CHLORIDE                                                  100HSO
E 000067481 0001
E 02 005412 022865

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N 000067561  METHANOL, SYNTHETIC                                              6060.1 MIL LBS  T72  MISC CHEMS           987.7 MIL LB
N 000067561 METHANOL                                                              CT
N 000067561 METHYL ALCOHOL                                                        DC
N 000067561 METHYL ALCOHOL                                                        FR
N 000067561 METHYL ALCOHOL                                                        FR
N 000067561 MX8048199                                                             MX
N 000067561 METHANOL                                                          171KSO
N 000067561 METHYL ALCOHOL                                                       FDA
N 000067561 METHYL ALCOHOL                                                        DC
N 000067561 METHANOL                                                              DC
N 000067561 MX8011458                                                             MX
N 000067561                                                                      CEH
N 000067561 MX8013658                                                             MX
N 000067561 MX8013523                                                             MX
N 000067561 MX8013669                                                             MX
N 000067561 MX8006073                                                             MX
N 000067561 METHYL ALCOHOL                                                       KEM
```

Table 3-3 (continued)

```
N 000067561
E 000067561 0001
E 05 004630 013911 016090 019064 019340

-------------------------------------------------------------------------------------------------------------------------------------

N 000067630  ISOPROPYL ALCCHCL                                              1790.0 MIL LBS  T72  MISC CHEMS          876.2 MIL LB
N 000067630 ISOPROPYL ALCCHCL                                                   FR
N 000067630 ISOPRCPANCL                                                         CT
N 000067630 ISCPROPYL ALCOHOL                                                   DC
N 000067630
N 000067630 ISOPROPYL ALCOHOL                                                  KEM
N 000067630 ISOPRCPANCL                                                         NP
N 000067630 ISOPROPYL ALCOHOL                                                   NP
N 000067630 MX8013534                                                           MX
N 000067630 MX8013670                                                           MX
N 000067630 MX8013681                                                           MX
N 000067630 MX8013692                                                           MX
N 000067630 MX8013705                                                           MX
N 000067630                                                                    CEH
N 000067630 MX8011469                                                           MX
N 000067630 ISOPROPYL ALCOHOL                                                   SF
N 000067630 ISOPROPYL ALCOHOL (ISOPRCPANOL)                                     FC
N 000067630 ISOPROPYL ALCOHCL                                                   FC
N 000067630 ISOPROPANCL (ISOPPOPYL ALCOHOL)                                     FC
N 000067630 ISOPRCPANCL                                                        FDA
N 000067630 MX8048202                                                           MX
N 000067630 MX8022626                                                           MX
N 000067630 MX8023094                                                           MX
N 000067630 MX8052333                                                           MX
N 000067630 ISOPROPYL ALCCHCL                                               272ISO
N 000067630 ISOPROPYL ALCOHOL                                                   FA
N 000067630 ISOPROPYL ALCOHCL                                                   HA
N 000067630 ISO-PRCPYL ALCCHCL (ISO-PRCPANOL)                                   FA
E 000067630 0001
E 05 015656 015685 016090 017841 019340

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N 000067641  ACETONE                                                        1704.1 MIL LBS  SRI  MISC CHEMS          533.9 MIL LB
N 000067641 ACETONE                                                             FA
N 000067641 MX8052173                                                           MX
N 000067641 ACETONE                                                         104ESO
N 000067641 ACETONE                                                             FC
N 000067641                                                                    CEH
N 000067641 MX8021850                                                           MX
N 000067641 MX8013658                                                           MX
N 000067641 MX8030339                                                           MX
N 000067641 DIMETHYL KETONE (ACETONE)                                          KEM
N 000067641 ACETONE                                                             NP
N 000067641 ACETCNE                                                 107 91  97 39
N 000067641 MX8003154                                                           MX
N 000067641 ACETONE                                                             DC
N 000067641 ACETONE                                                             CT
N 000067641
E 000067641 0001
E 13 004492 004630 004918 005975 009487 011162 013030 014210 015334 015656 017758 019834 021337
```

Table 3-3 (continued)

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N 000067663  CHLOROFORM                                                      234.7 MIL LBS  T72  MISC CHEMS         167.8 MIL LB
N 000067663 CHLOROFORM                                                          CD
N 000067663 CHLOROFORM                                                          CT
N 000067663 CHLOROFORM                                             125113   66 66
N 000067663 CHLOROFORM                                                          DC
N 000067663 CHLOROFORM                                                          NP
N 000067663                                                                    CEH
N 000067663 CHLOROFORM                                                      141KSO
N 000067663 CHLOROFORM                                                           P
N 000067663 MX8061618                                                           MX
N 000067663
E 000067663 0001
E 08 004615 004630 006978 010817 012940 018911 021321 021994

------------------------------------------------------------------------------------------------------------------------------

N 000068268  VITAMIN A                                                         1.0 MIL LBS  T72  MEDICINAL CHEMS
N 000068268
N 000068268 MX8001692                                                           MX
N 000068268 MX8006982                                                           MX
N 000068268 MX8017309                                                           MX
N 000068268 MX8021792                                                           MX
N 000068268 MX8059301                                                           MX
N 000068268 MX8059027                                                           MX
N 000068268 MX8059049                                                           MX
N 000068268 MX8017707                                                           MX
N 000068268                                                                    CEH
N 000068268 MX8017296                                                           MX
N 000068268 MX8059298                                                           MX
N 000068268 MX8017310                                                           MX
N 000068268 MX8048928                                                           MX
N 000068268 MX8026731                                                           MX
N 000068268 MX8026640                                                           MX
N 000068268 MX8026344                                                           MX
N 000068268 MX8026355                                                           MX
N 000068268 MX8026322                                                           MX
N 000068268 MX8028113                                                           MX
N 000068268 MX8028146                                                           MX
N 000068268 MX8026333                                                           MX
N 000068268 MX8028157                                                           MX
N 000068268 MX8026617                                                           MX
N 000068268 MX8043423                                                           MX
N 000068268 MX8026491                                                           MX
N 000068268 MX9026639                                                           MX
N 000068268 MX8026742                                                           MX
N 000068268 MX8027698                                                           MX
N 000068268 MX8013147                                                           MX
N 000068268 MX8027585                                                           MX
N 000068268 MX8043412                                                           MX
N 000068268 MX8028124                                                           MX
N 000068268 MX8026468                                                           MX
N 000068268 MX8013716                                                           MX
N 000068268 MX8028044                                                           MX
N 000068268 MX8027654                                                           MX
```

Table 3-3 (continued)

```
N 000068268 MX8027665                                                    MX
N 000068268 VITAMIN A                                                    FC
N 000068269 VITAMIN A                                                    DC
N 000068268 VITAMIN A                                                    NP
N 000068268 VITAMIN A                                                     C
N 000068268 VITAMIN A                                             09849  CEH
N 000068268 VITAMIN A                                                    FA
N 000068268 MX8057554                                                    MX
N 000068268 MX8058400                                                    MX
N 000068268 MX8055569                                                    MX
N 000068268 MX8058024                                                    MX
N 000068268 MX8058411                                                    MX
N 000068268 MX8054635                                                    MX
N 000068268 MX8026286                                                    MX
N 000068268 MX8026311                                                    MX
N 000068268 MX8048406                                                    MX
N 000068269 VITAMIN A                                                040ASO
N 000068268 MX8026264                                                    MX
N 000068268 MX8026242                                                    MX
N 000068268 MX8047970                                                    MX
N 000068268 MX8026253                                                    MX
N 000068268 VITAMIN A, NATURAL                                           PD
N 000068268 VITAMIN A                                                    PD
E 000068268 0001
E 09 008023 009538 010902 011780 013212 013769 015307 020228 022847

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N 000069727  SALICYLIC ACID                                             8.7 MIL LBS  T72  MEDICINAL CHEMS
N 000069727 MX8013738                                                    MX
N 000069727 MX8013625                                                    MX
N 000069727                                                             CEH
N 000069727 MX8007805                                                    MX
N 000069727 MX8012406                                                    MX
N 000069727 SALICYLIC ACID                                               NP
N 000069727 SALICYLIC ACID                                               DC
N 000069727 MX8047709                                                    MX
N 000069727 008060502                                                    MX
N 000069727 SALICYLIC ACID                                               PD
N 000069727 MX8054931                                                    MX
N 000069727 MX8052311                                                    MX
N 000069727 MX8056880                                                    MX
N 000069727 SALICYLIC ACID                                           111BSO
N 000069727
N 000069727 SALICYLIC ACID                                               CT
N 000069727  SALICYLIC ACID, TECH.                                     47.1 MIL LBS  T72  CYCLIC INTERMED
E 000069727 0001
E 04 004616 009270 020992 021337

--------------------------------------------------------------------------------------------------

N 000071238  PROPYL ALCCHOL (PRCPANCL)                                 83.1 MIL LBS  T72  MISC CHEMS          63.6 MIL LB
N 000071238 PRCPANCL                                                     CT
N 000071238 PROPYL ALCCHOL                                               DC
N 000071238 NORMAL PRCPYL ALCOHCL                                       KEM
N 000071238 PROPYL ALCOHOL                                               SF
N 000071238                                                             CEH
```

Table 3-3 (continued)

```
N 000071238 PROPYL ALCCHOL                                         FC
N 000071238 PROPYL ALCOHOL (PROPANOL)                              FA
N 000071238 N-PROPYL ALCOHCL                                       FA
N 000071238 PROPYL ALCCHCL                                     283JSO
N 000071238
E 000071238 0001
E 03 004630 005961 016090

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N 000071363  N-BUTYL ALCCHCL                                    590.2 MIL LBS  T72  MISC CHEMS          144.6 MIL LB
N 000071363 BUTYL ALCOHOL                                         FDA
N 000071363 MX8023129                                              MX
N 000071363 MX8025216                                              MX
N 000071363 BUTYL ALCOHOL                                      251HSO
N 000071363 N-BUTYL ALCCHCL                                        FA
N 000071363 N-BUTANOL                                              CT
N 000071363 BUTYL ALCOHOL, NORMAL                                  DC
N 000071363 N-BUTYL ALCOHOL                                        FR
N 000071363 BUTANOL                                                CT
N 000071363                                                       CEH
N 000071363 BUTYL ALCCHCL                                          FC
N 000071363 BUTYL ALCOHOL                                          SF
N 000071363 N-BUTANOL                                             KEM
N 000071363
E 000071363 0001
E 04 004630 010848 016373 021337

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N 000071432  BENZENE                                           8937.1 MIL LBS  T72  CRUDE PRODUCTS      183.6 MIL LB
N 000071432 BENZENE                                            091GSO
N 000071432 BENZOL (BENZENE)                                       PR
N 000071432 AROMATICS %E.G. BENZENE<                               CT
N 000071432 BENZENE                                                DC
N 000071432 BENZENE                                                CT
N 000071432 BENZENE                                                CT
N 000071432 BENZENE                                                FR
N 000071432 BENZENE                                     229278 284175
N 000071432                                                       CEH
N 000071432 BENZENE                                               KEM
N 000071432 MX8007452                                              MX
N 000071432
E 000071432 0003
E 18 004629 004630 004762 004800 004845 004846 004847 004850 004859 005964 006386 006400 006584 007092 007308 007729 007871 007993
E 18 008846 009526 010254 011273 011885 012722 012912 012940 012970 013307 014737 014814 015408 015424 016030 018215 018446 018882
E 05 019405 020447 020657 021380 021381

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N 000072435  METHOXYCHLCR                                       10.0 MIL LBS  SRI  PESTICIDES
N 000072435 METHCXYCHLCR                                           CT
N 000072435 MX8026366                                              MX
N 000072435                                                       CEH
N 000072435 METHCXYCHLCP                                            P
```

Table 3-3 (continued)

```
N 000072435
E 000072435 0001
F 04 006618 013248 014190 022864

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N 000074317  N,N'-DIPHENYL-P-PHENYLENEDIAMINE                                  1.8 MIL LBS  T72  RUBBER PROC CHEMS
N 000074317
N 000074317 N,N'-DIPHENYL-P-PHENYLENECIAMINE                                071FSO
N 000074317 N,N'-DIPHENYL-P-PHENYLENECIAMINE                                   FDA
N 000074317                                                                    CEH
N 000074317 N,N'-DIPHENYL-P-PHENYLENEDIAMINE                                353244
F 000074317 0001
E 01 009991

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N 000074839  METHYL BRCMIDE                                                   24.6 MIL LBS  T72  PESTICIDES          22.4 MIL LB
N 000074839 METHYL BRCMIDE                                                      CT
N 000074839 BROMIDES (E.G. METHYL BROMIDE)                                      FR
N 000074839 MX8000224                                                           MX
N 000074839 MX8000213                                                           MX
N 000074839 MX8004099                                                           MX
N 000074839 METHYL BRCMIDE                                                       P
N 000074839 BROMOMETHANE                                                    132JSO
N 000074839
E 000074839 0001
E 01 019016

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N 000074840  ETHANE                                                         5136.5 MIL LBS  T72  CRUDE PRODUCTS      51.4 MIL LB
N 000074840 ETHANE                                                          069ASC
N 000074840 MX8006142                                                           MX
N 000074840
E 000074840 0001
E 02 011707 012699

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N 000074851  ETHYLENE                                                      20852.1 MIL LBS  T72  CRUDE PRODUCTS     521.3 MIL LB
N 000074851
N 000074851 OLEFINS (C2, C3-C12) (E.G. ETHYLENE)                                FR
N 000074851                                                                    CEH
N 000074851 ETHYLENE                                                        159ISO
E 000074851 0001
E 08 010346 012699 013360 014693 014881 016767 017134 017589

------------------------------------------------------------------------------------------------------------------------------

N 000074873  CHLCRCMETHANE (METHYL CHLCRIDE)                                 453.5 MIL LBS  T72  MISC CHEMS          18.1 MIL LB
```

Table 3-3 (continued)

```
N 000074873
N 000074873 METHYL CHLORIDE                                          CEH
N 000074873 CHLOROMETHANE                                            DC
N 000074873                                                      142ASO
E 000074873 0001
E 02 010868 022871

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N 000074884  IODOMETHANE (METHYL IODIDE)
N 000074884                                                 18.0 MIL LBS  T72  MISC CHEMS
N 000074884 IODOMETHANE
N 000074884                                                  271CSO
N 000074884 IODOMETHANE                                        CEH
E 000074884 0001                                        189    112
E 05 007887 008065 014842 020273 021337

--------------------------------------------------------------------------------

N 000074895  MONOMETHYLAMINE
N 000074895                                                 33.1 MIL LBS  T72  MISC CHEMS
N 000074895 METHYLAMINE                                     CEH
N 000074895                                                173BSC
E 000074895 0001
E 05 008273 011707 012699 014361 017886

--------------------------------------------------------------------------------

N 000074986  PROPANE
N 000074986                                              9608.3 MIL LBS  T72  CRUDE PRODUCTS      96.1 MIL LB
N 000074986 PROPANE
N 000074986 PROPANE                                       184HSO
N 000074986 PROPANE                                           FA
N 000074986 PROPANE                                           PR
N 000074986 MX8006142                                         FC
E 000074986 0001                                              MX
E 01 012699

--------------------------------------------------------------------------------

N 000075014  VINYL CHLORIDE, MONOMER (CHLOROETHYLENE)
N 000075014                                              5088.5 MIL LBS  T72  MISC CHEMS        146.5 MIL LB
N 000075014
N 000075014 MX8013772                                        CEH
N 000075014 CHLOROETHYLENE                                    MX
N 000075014 VINYL CHLORIDE                                141JSC
E 000075014 0002                                              CT
E 18 018068 020026 020040 020058 020131 020152 020315 020649 020670 020756 020853 020989 021076 021337 021339 021342 021347 021916
E 08 021972 021990 021995 021996 022339 022369 022870 022871

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```

Table 3-3 (continued)

```
N 000075047  ETHYLAMINE, MONC                                          45.9 MIL LBS  SRI  MISC CHEMS          14.4 MIL LB
N 000075047 ETHYLAMINE                                               159CSO
N 000075047                                                             CEH
N 000075047
E 000075047 0001
E 04 005412 017493 017886 019343

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N 000075070  ACETALCEHYCE                                            1447.6 MIL LBS  T72  MISC CHEMS          36.2 MIL LB
N 000075070 ACETALDEHYDE                                             103DSO
N 000075070 ACETALDEHYCE (ETHANAL)                                       FA
N 000075070 ACETALCEHYDE                                                 PR
N 000075070                                                             CEH
N 000075070 MX8006904                                                    MX
N 000075070 ACETALDEHYDE                                                 SF
N 000075070 ACETALDEHYCE                                                 FC
N 000075070 MX8008513                                                    MX
N 000075070
E 000075070 0001
E 01 004918

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N 000075150  CARBON DISULFIDE                                         767.8 MIL LBS  T72  MISC CHEMS          49.9 MIL LB
N 000075150
N 000075150                                                             CEH
N 000075150 CARBON CISULFIDE                                             DC
N 000075150 CARBON DISULFIDE (CARBON CISULPHICE)                         CT
N 000075150 CARBON DISULFIDE                                              P
N 000075150 CARBON DISULFIDE                                         138FSO
E 000075150 0001
E 01 018805

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N 000075218  ETHYLENE OXIDE                                          3961.8 MIL LBS  T72  MISC CHEMS          98.8 MIL LB
N 000075218                                                             CEH
N 000075218 ETHYLENE OXIDE                                               FC
N 000075218 MX8012428                                                    MX
N 000075218 MX8013794                                                    MX
N 000075218 MX8013783                                                    MX
N 000075218 MX8013807                                                    MX
N 000075218 MX8013829                                                    MX
N 000075218 MX8013819                                                    MX
N 000075218 ETHYLENE CXIDE                                           160CSC
N 000075218 ETHYLENE OXIDE                                                P
N 000075218
N 000075218 ETHYLENE CXIDE                                                C
E 000075218 0004
E 18 004535 004641 004542 004925 004946 004993 005044 005131 005106 005145 005379 005606 005782 005783 006304 006591 006917 007049
E 18 007357 009410 009488 009557 010579 010610 010759 010790 010855 010863 010868 011041 011473 011803 011883 012682 013098 013279
E 18 013400 014069 015857 015869 016040 016515 017582 017990 018448 020122 020471 020580 020815 021483 021748 021770 021877 021878
E 01 021901
```

Table 3-3 (continued)

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N 000075569  PROPYLENE OXIDE                                          1640.0 MIL LBS  T72  MISC CHEMS         40.8 MIL LB
N 000075569
N 000075569 PROPYLENE OXIDE                                               CT
N 000075569 PROPYLENE OXIDE                                           185JSO
N 000075569 PROPYLENE OXIDE                                                P
N 000075569                                                              CEH
N 000075569 PROPYLENE OXIDE                                               FC
E 000075569 0001
E 11 004993 005000 005063 008407 009179 010869 011883 012998 013215 019048 021077

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N 000075605  DIMETHYLARSENIC ACID (CACODYLIC ACID)                       2.0 MIL LBS  SRI  PESTICIDES
N 000075605 HYDROXYDIMETHYLARSINE OXIDE                               137MSO
N 000075605 CACODYLIC ACID                                                 P
N 000075605                                                              CEH
N 000075605 HYDROXYDIMETHYLARSINE OXIDE                               109
N 000075605
E 000075605 0001
E 03 013029 014733 022878

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N 000075650  TERT-BUTYL ALCOHOL                                       1000.0 MIL LBS  SRI  MISC CHEMS        715.0 MIL LB
N 000075650                                                              CEH
N 000075650 TERTIARY BUTYL ALCOHOL                                       KEM
N 000075650 TERT-BUTYL ALCOHOL                                        251JSO
N 000075650
E 000075650 0001
E 07 004630 009487 010843 011162 013911 017495 019340

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N 000075694  TRICHLOROFLUOROMETHANE                                    299.6 MIL LBS  T72  MISC CHEMS        274.1 MIL LB
N 000075694
N 000075694 TRICHLOROFLUOROMETHANE                                    192ESC
N 000075694                                                              CEH
N 000075694 FREON 11                                                      CT
N 000075694 FREON 11                                                       C
N 000075694 TRICHLOROFLUOROMETHANE                                         C
N 000075694 TRICHLOROMONOFLUOROMETHANE                                    CT
N 000075694 FREON 11                                                      FR
N 000075694 FREON 11                                                      FR
E 000075694 0001
E 01 021994

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```

Table 3-3 (continued)

```
N 000075718  DICHLORODIFLUOROMETHANE                                         439.2 MIL LBS  T72  MISC CHEMS        401.9 MIL LB
N 000075718
N 000075718                                                                  CEH
N 000075718 FREON 12                                                          FR
N 000075718 FREON 12                                                          FR
N 000075718 DICHLORODIFLUOROMETHANE                                           CT
N 000075718 FREON 12                                                           C
N 000075718 PROPELLANT 12                                                     CT
N 000075718 FREON 12                                                          CT
N 000075718 DICHLORODIFLUOROMETHANE                                        26FSC
E 000075718 0001
E 02 012715 018212

-------------------------------------------------------------------------------------------------------------------------------

N 000076448  HEPTACHLOR                                                        6.0 MIL LBS  SRI  PESTICIDES
N 000076448                                                                  CEH
N 000076448
N 000076448 1,4,5,6,7,8,8-HEPTACHLORO-3A.4.-7,7A-TETRAHYDRO-4,7-METHANOIDENE  2GSD
N 000076448 HEPTACHLOR                                                         P
N 000076448 HEPTACHLOR                                                        CT
E 000076448 0001
E 10 006618 009044 010806 011498 011722 012984 013610 021385 022818 022827

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N 000077929  CITRIC ACID                                                     163.0 MIL LBS  SRI  MISC CHEMS        119.2 MIL LB
N 000077929
N 000077929 CITRIC ACID                                                       NP
N 000077929 CITRIC ACID                                                       DC
N 000077929 CITRIC ACID                                                       NP
N 000077929 MX8017456                                                         MX
N 000077929 CITRIC ACID                                                       FC
N 000077929 CITRIC ACID                                                       FC
N 000077929 CITRIC ACID                                                       FC
N 000077929 CITRIC ACID                                                       FC
N 000077929 CITRIC ACID                                                       SF
N 000077929 MX8006164                                                         MX
N 000077929 MX8006119                                                         MX
N 000077929 MX8006175                                                         MX
N 000077929 MX8006153                                                         MX
N 000077929 MX8003109                                                         MX
N 000077929 MX8027530                                                         MX
N 000077929 MX8013874                                                         MX
N 000077929 MX8013896                                                         MX
N 000077929 MX8046671                                                         MX
N 000077929 MX8030442                                                         MX
N 000077929 MX8031309                                                         MX
N 000077929 MX8027461                                                         MX
N 000077929 MX8028566                                                         MX
N 000077929 MX8028588                                                         MX
N 000077929 MX8030840                                                         MX
N 000077929 MX8013885                                                         MX
N 000077929 MX8012393                                                         MX
N 000077929 MX8050871                                                         MX
N 000077929 MX8012280                                                         MX
N 000077929 CITRIC ACID, ANHYDROUS                                            CD
```

Table 3-3 (continued)

```
N 000077929 CITRIC ACID                                            CT
N 000077929 CITRIC PECTIN                                           C
N 000077929 ORGANIC ACIDS %E.G. CITRIC<                            CT
N 000077929 CITRIC ACID                                            FA
N 000077929 CITRIC ACID                                        145BSO
N 000077929 MX8061618                                              MX
N 000077929 MX8060740                                              MX
N 000077929 MX8058035                                              MX
N 000077929 MX8053529                                              MX
N 000077929 MX8052957                                              MX
N 000077929 MX8052220                                              MX
N 000077929 MX8056891                                              MX
N 000077929 MX8023276                                              MX
N 000077929 MX8048495                                              MX
N 000077929 MX8023618                                              MX
N 000077929 MX8048508                                              MX
N 000077929 MX8022648                                              MX
N 000077929 MX8023583                                              MX
E 000077929 0001
E 01 008904

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N 000078831  ISOBUTYL ALCOHOL (ISOPROPYL CARBINOL)                 96.4 MIL LBS  T72  MISC CHEMS        29.5 MIL LB
N 000078831
N 000078831 ISOBUTYL ALCOHOL                                       FC
N 000078831 ISOBUTYL ALCOHOL                                      KEM
N 000078831 ISOBUTYL ALCOHOL                                       SF
N 000078831 ISOBUTANOL                                             CT
N 000078831 ISOBUTYL ALCOHOL                                       DC
N 000078831 ISOBUTYL ALCOHOL                                   271ISO
N 000078831 ISO-BUTYL ALCOHOL (ISO-BUTANOL)                        FA
E 000078831 0001
E 02 004630 0

-------------------------------------------------------------------------------------------------------------

N 000078933  2-BUTANONE (METHYL ETHYL KETONE)                     509.0 MIL LBS  T72  MISC CHEMS       524.7 MIL LB
N 000078933 METHYL ETHYL KETONE                                    FR
N 000078933
N 000078933 METHYL ETHYL KETONE                                    CT
N 000078933 KETONES %E.G. METHYL ETHYL DETONE<                     CT
N 000078933 METHYL ETHYL KETONE (MEK)                             KEM
N 000078933                                                       CEH
N 000078933 2-BUTANONE                                             FC
N 000078933 METHYL ETHYL KETONE                                    DC
N 000078933 2-BUTANONE                                             SF
N 000078933 2-BUTANONE                                             FA
N 000078933 2-BUTANONE                                         251CSO
N 000078933 METHYL ETHYL KETONE (2-BUTANONE)                       FA
E 000078933 0001
E 01 004918

-------------------------------------------------------------------------------------------------------------
```

Table 3-3 (continued)

```
N 000079016  TRICHLOROETHYLENE                              426.7 MIL LBS  T72  MISC CHEMS        429.5 MIL LB
N 000079016                                                   CEH
N 000079016 TRICHLOROETHYLENE                                 FC
N 000079016 TRICHLOROETHYLENE                                 DC
N 000079016 TRICHLOROETHYLENE                                 KEM
N 000079016 TRICHLOROETHYLENE                              192DSO
N 000079016 TRICHLOROETHYLENE                                  P
N 000079016 TRICHLOROETHYLENE                                 PD
N 000079016
N 000079016 TRICHLOROETHYLENE                                 CT
N 000079016 TRICHLOROETHYLENE                                 FR
N 000079016 TRICHLOROETHYLENE                                 FR
E 000079016 0001
E 0[illegible] 004630 021321 021339 021978

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N 000079094  PROPIONIC ACID                                  56.0 MIL LBS  T72  MISC CHEMS
N 000079094
N 000079094                                                   CEH
N 000079094 PROPIONIC ACID                                    FC
N 000079094 ETHYL FORMIC ACID (PROPIONIC ACID)                FC
N 000079094 PROPIONIC ACID                                    FC
N 000079094 PROPIONIC ACID                                    NP
N 000079094 PROPIONIC ACID                                 283FSO
N 000079094 PROPIONIC ACID                                    FA
E 000079094 0001
E 03 004616 005412 012992

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N 000079107  ACRYLIC ACID                                   123.2 MIL LBS  T72  MISC CHEMS
N 000079107 ACRYLIC ACID                                  117ASC
N 000079107 ACRYLIC ACID                                      PR
N 000079107                                                   CEH
N 000079107
E 000079107 0001
E 01 004616

-------------------------------------------------------------------------------------------------------------------

N 000080057  4,4'-ISOPROPYLIDENEDIPHENOL (BISPHENOL A)       255.2 MIL LBS  T72  CYCLIC INTERMED
N 000080057 BISPHENOL A                                       CT
N 000080057 4,4'-ISOPROPYLIDENEDIPHENOL                   087ESC
N 000080057                                                   CEH
N 000080057 MX8030315                                         MX
N 000080057
F 000080057 0001
E 01 020523

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N 000080433  DICUMYL PEROXIDE                                15.0 MIL LBS  SRI  RUBBER-PROC CHEM   15.3 MIL LB
```

Table 3-3 (continued)

```
N 000080433 BIS(ALPHA,ALPHA-DIMETHYLBENZYL)PEROXIDE                     250GSO
N 000080433 DICUMYL PERCXIDE                                               FDA
N 000080433 DICUMYL PEROXIDE                                               FDA
N 000080433
N 000080433                                                                CEH
E 000080433 0001
E 01 010642

------------------------------------------------------------------------------------------------

N 000080626  METHYL METHACRYLATE
N 000080626                                                        599.0 MIL LBS  T72  MISC CHEMS
N 000080626 METHYL METHACPYLATE MCNCMER                                     CT
N 000080626 RESINS, SYNTHETIC %E.G. EMTHYL METHALRYLATE<                    CT
N 000080626 METHYL METHACRYLATE                                             CT
N 000080626 MX8063454                                                       MX
N 000080626 METHACRYLIC ACID, METHYL ESTER                              275HSO
N 000080626 METHYL METHACRYLATE                                            FDA
N 000080626 MX8013921                                                       MX
E 000080626 0001
E 01 019448

------------------------------------------------------------------------------------------------

N 000081072  SACCHARIN
N 000081072                                                          4.8 MIL LBS  SRI  FLAVOR & PERFUME
N 000081072 SACCHARIN (2,3-DIHYDRO-3-OXO-BENZISOSULFONAZOLE)               CEH
N 000081072 SACCHARIN                                                       FC
N 000081072 MX8028920                                                       DC
N 000081072 MX8013567                                                       MX
N 000081072 SACCHARIN                                                       MX
N 000081072 1,2-BENZISOTHIAZOLIN-3-ONE,1,1-DIOXIDE                          NP
N 000081072 AMMONIUM SACCHARIN                                          093ASO
N 000081072 CALCIUM SACCHARIN                                               FA
N 000081072 MX8060546                                                       FA
N 000081072 MX8052775                                                       MX
N 000081072 SACCHARIN                                                       MX
N 000081072 SACCHARIN                                                       FA
N 000081072 MX8022591                                                       PD
N 000081072 SACCHARIN                                                       MX
N 000081072                                                                 CT
E 000081072 0001
E 01 020267

------------------------------------------------------------------------------------------------

N 000081492  1-AMINO-2,4-DIBROMOANTHRAQUINONE
N 000081492                                                          1.0 MIL LBS  T72  CYCLIC INTERMED
N 000081492
N 000081492 1-AMINO-2,4-DIBROMOANTHRAQUINONE                               CEH
E 000081492 0001                                                        322CSO
E 01 022863

------------------------------------------------------------------------------------------------
```

Table 3-3 (continued)

```
N 000081641  1,4-DIHYDROXYANTHRAQUINONE (QUINIZARIN)                            2.1 MIL LBS  T72  CYCLIC INTERMED
N 000081641                                                                    CEH
N 000081641
N 000081641 1,4-DIHYDROXYANTHRAQUINONE                                      240JSO
E 000081641 0001
E 03 010570 012421 022863

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N 000081812  WARFARIN                                                          12.0 MIL LBS  SRI  PESTICIDES
N 000081812                                                                    CEH
N 000081812 COUMADIN                                                            PA
N 000081812
N 000081812 WARFARIN                                                            FR
N 000081812 WARFARIN                                                             P
N 000081812 3-(ALPHA-ACETONYLBENZYL)-4-HYDROXYCOUMARIN                      290ASO
N 000081812 COUMADIN                                                            HA
E 000081812 0001
E 01 009147

------------------------------------------------------------------------------------------------------------------------------------

N 000082053  7H-BENZ(DE)ANTHRACEN-7-ONE (BENZANTHRONE)                          1.2 MIL LBS  T72  CYCLIC INTERMED
N 000082053                                                                    CEH
N 000082053 7H-BENZ(DE)ANTHRACEN-7-ONE                                      096BSO
N 000082053
N 000082053 7 H BENZ(DE)ANTHRACENE-7-ONE                                        FR
E 000082053 0001
E 02 012984 022863

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N 000082688  PENTACHLORONITROBENZENE (PCNB)                                     3.0 MIL LBS  SRI  PESTICIDES
N 000082688
N 000082688                                                                    CEH
N 000082688 PENTACHLORONITROBENZENE                                           290
N 000082688 MX8003212                                                           MX
N 000082688 PCNB                                                                 P
N 000082688 PENTACHLORONITROBENZENE                                         100ASO
E 000082688 0001
E 10 008085 008833 011756 017636 020299 020762 021385 022827 022877 022878

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N 000084662  DIETHYL PHTHALATE                                                 19.0 MIL LBS  T72  PLASTICIZERS         19.3 MIL LB
N 000084662 PHTHALIC ACID, DIETHYL ESTER                                    282HSO
N 000084662                                                                    CEH
N 000084662 DIETHYL PHTHALATE                                                   DC
N 000084662 DIETHYL PHTHALATE                                                   CT
N 000084662
E 000084662 0001
```

Table 3-3 (continued)

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E 01 005412

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N 000084742  DIBUTYL PHTHALATE                                                 29.1 MIL LBS  T72  PLASTICIZERS          29.5 MIL LB
N 000084742                                                                     CEH
N 000084742 DIBUTYL PHTHALATE                                                   KEM
N 000084742 DIBUTYL PHTHALATE                                                    DC
N 000084742
N 000084742 DIBUTYL PHTHALATE                                                    CT
N 000084742 DIBUTYL PHTHALATE                                                    AR
N 000084742 PHTHALIC ACID, DIBUTYL ESTER                                     183ESO
E 000084742 0001
E 02 012917 018783

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N 000086306  N-NITROSODIPHENYLAMINE                                             2.0 MIL LBS  T72  RUBBER PROC CHEMS
N 000086306 N-NITROSODIPHENYLAMINE                                           279KSO
N 000086306 N-NITROSODIPHENYLAMINE                                             284
N 000086306                                                                     CEH
E 000086306 0001
E 07 005412 008323 008324 008333 008517 017876 021337

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N 000086500  AZINPHOSMETHYL                                                     4.0 MIL LBS  SRI  PESTICIDES
N 000086500 AZINPHOSMETHYL                                                        P
N 000086500 GUTHION (METHYL GUTHION)                                              P
N 0000865001P(O-METHYL)-1,2,3-BENZOTRIAZIN-4(3H)-ONE                         091ESO
N 000086500 PHOSPHORODITHIOIC ACID,O,C-DIMETHYL ESTER, S-ESTER WITH 3-(MERCA091FSC
N 000086500                                                                     CEH
N 000086500
E 000086500 0001
E 05 018192 021410 021458 022877 022878

--------------------------------------------------------------------------------------------------------------------------

N 000087865  PENTACHLOROPHENOL (PCP)                                           49.7 MIL LBS  T72  PESTICIDES
N 000087865                                                                     CEH
N 000087865 PENTACHLOROPHENOL                                        331       291
N 000087865 PENTACHLOROPHENOL                                                   KEM
N 000087865 PENTACHLOROPHENOL                                                071GSO
N 000087865 PENTACHLOROPHENOL                                                     P
N 000087865 PENTACHLOROPHENOL                                                     P
N 000087865 PCP                                                                   P
N 000087865 PENTACHLOROPHENOL                                                    CT
N 000087865 PENTACHLOROPHENOL                                                    FR
N 000087865
E 000087865 0001
E 06 005681 006630 009542 013029 014101 020762
```

Table 3-3 (continued)

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N 000088857  DINITROBUTYLPHENOL (DNBP)                                            3.0 MIL LBS   SRI  PESTICIDES
N 000088857 2-SEC-BUTYL-4,6-DINITROPHENOL                                     136ASD
N 000088857 DNBP                                                                   P
N 000088857                                                                      CEH
N 000088857 2-SEC-BUTYL-4,6-DINITROPHENOL                          301    191
N 000088857
E 000088857 0001
E 03 013029 014531 022878

--------------------------------------------------------------------------------------------------------------------------------

N 000093710  2-CHLORO-N,N-DIALLYACETAMIDE (CDAA)                                 10.0 MIL LBS   SRI  PESTICIDES
N 000093710                                                                      CEH
N 000093710 MX8005434                                                             MX
N 000093710 MX8003289                                                             MX
N 000093710 CDAA                                                                   P
N 000093710 CDAA (RANDOX)                                                          P
N 000093710 RANDOX                                                                 P
N 000093710
N 000093710 N,N-DIALLYL-2-CHLOROACETAMIDE                                     438FSD
N 000093710 CDAA                                                                  FR
E 000093710 0001
E 01 013029

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N 000093721  2-(2,4,5-TRICHLOROPHENOXY)PROPIONIC ACID (SILVEX)                    3.0 MIL LBS   SRI  PESTICIDES
N 000093721
N 000093721 SILVEX                                                                 P
N 000093721 TRICHLOROPHENATES (E.G. 2,4,5 TRICHLOROPHENOXY PROPIONIC ACID          P
N 000093721 SILVEX                                                                 P
N 000093721 2-(2,4,5-TRICHLOROPHENOXY)PROPIONIC ACID                          193DSD
N 000093721 MX8053212                                                             MX
N 000093721 2-(2,4,5-TRICHLOROPHENOXY)PROPIONIC ACID                            317
N 000093721                                                                      CEH
E 000093721 0001
E 02 013029 015665

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N 000093765  2,4,5-TRICHLOROPHENOXYACETIC ACID ESTERS & SALTS                <    5.0 MIL LBS   SRI  PESTICIDES
N 000093765
N 000093765 2,4,5-T (2,4,5-TRICHLOROPHENOXYACETIC ACID)                            P
N 000093765 2,4,5-TRICHLOROPHENOXY ACETIC ACID (2,4,5-T ACID)                      P
N 000093765 (2,4,5-TRICHLOROPHENOXY)ACETIC ACID                               193ASD
N 000093765 MX8053212                                                             MX
N 000093765 MX8063727                                                             MX
N 000093765                                                                      CEH
N 000093765 (2,4,5-TRICHLOROPHENOXY)ACETIC ACID                    450    316
N 000093765 MX8015358                                                             MX
E 000093765 0002
E 18 005404 005760 007259 007874 009262 009542 011141 011158 011198 012006 012939 013002 013029 014070 014101 014387 015665 015921
```

Table 3-3 (continued)

```
E 10 016741 018201 018295 018686 020055 020762 021385 022812 022827 022897

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N 000094360  BENZOYL PEROXIDE                                                     7.6 MIL LBS  T72  MISC CHEMS
N 000094360 BENZOYL PEROXIDE                                                  129GSO
N 000094360 PEROXIDE, BENZOYL                                                     FA
N 000094360 BENZCYL PERCXIDE                                                      PD
N 000094360 BENZOYL PEROXICE                                                      DC
N 000094360 BENZCYL PEROXIDE                                                      CT
N 000094360                                                                      CEH
N 000094360 BENZOYL PEROXIDE                                                      NP
N 000094360 BENZOYL PERCXIDE                                                      FC
N 000094360
E 000094360 0001
E 03 004616 011162 012984

------------------------------------------------------------------------------------------------------------------------------------

N 000094757  2,4-DICHLOROPHENOXYACETIC ACID (2,4-D)                          <   40.0 MIL LBS  SRI  PESTICIDES
N 000094757
N 000094757 2,4-D                                                                  P
N 000094757 MX8063738                                                             MX
N 000094757 MX8053212                                                             MX
N 000094757 (2,4-DICHLOROPHENOXY)ACETIC ACID 2,4-D                            062ESO
N 000094757                                                                      CEH
N 000094757 MX8015358                                                             MX
N 000094757 (2,4-DICHLOROPHENOXY)ACETIC ACID                        261325 319220
N 000094757 MX8003289                                                             MX
N 000094757 MX8003325                                                             MX
N 000094757 2,4-DICHLCROPHENCXY ACETIC ACIC                               11512  CEH
E 000094757 0003
E 18 004616 004632 004688 005404 006473 006480 007874 008965 009192 009357 009542 011158 011198 011257 011500 011715 012313 012790
E 18 012983 012984 013029 013085 013662 014070 014124 014387 014486 014552 014881 015350 015665 016720 016741 017078 017487 017636
E 17 018162 018269 018373 020055 020142 020182 020313 020559 020573 020762 021385 021723 021799 022811 022812 022827 022897

------------------------------------------------------------------------------------------------------------------------------------

N 000095487  O-CRESOL                                                            49.7 MIL LBS  T72  CYCLIC INTERMED      15.6 MIL LB
N 000095487 ORTHO CRESOL                                                  3573   CEH
N 000095487                                                                      CEH
N 000095487 MX8003336                                                             MX
N 000095487 O-CRESOL                                                          214ESO
N 000095487
E 000095487 0001
E 02 010652 010781

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N 000095501  O-DICHLOROBENZENE                                                   62.4 MIL LBS  T72  CYCLIC INTERMED      27.1 MIL LB
N 000095501                                                                      CEH
N 000095501 ORTHO DICHLOROBENZENE                                                 DC
N 000095501 O-DICHLOROBENZENE                                                 216HSO
```

Table 3-3 (continued)

```
N 000095501 ORTHO DICHLOROBENZENE                                P
N 000095501
N 000095501 ORTHO DICHLOROBENZENE                     11485  CEH
N 000095501 O-DICHLOROBENZENE                                 CT
N 000095501 ORTHO-DICHLOROBENZENE                             CT
E 000095501 0001
E 04 004629 005170 005695 013029

---------------------------------------------------------------------------------------------------------

N 000095807  TOLUENE-2,4-DIAMINE (4-M-TOLYLENEDIAMINE)          167.9 MIL LBS  T72  CYCLIC INTERMED
N 000095807 TOLUENE-2,4-DIAMINE                              243BSC
N 000095807
N 000095807                                                     CEH
E 000095807 0001
E 01 021337

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N 000096128  1,2-DIBROMO-3-CHLOROPROPANE (DBCP)                  10.0 MIL LBS  SRI  PESTICIDES
N 000096128
N 000096128 NEMGAON (FUMAZONE, DIBROMOCHLOROPROPANE)                P
N 000096128 DICHLOROPROPANE                                         P
N 000096128 1,2-DIBROMO-3-CHLOROPROPANE                          9ASC
N 000096128                                                       CEH
N 000096128 NEMAGON                                               FR
E 000096128 0001
E 01 021927

---------------------------------------------------------------------------------------------------------

N 000098953  NITROBENZENE                                       551.2 MIL LBS  T72  CYCLIC INTERMED      19.3 MIL LB
N 000098953 NITROBENZENE                                         CT
N 000098953
N 000098953                                                       CEH
N 000098953 NITROBENZENE                                        234DSO
E 000098953 0001
E 03 004630 010783 018236

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N 000100425  STYRENE, ALL GRADES                               5940.7 MIL LBS  T72  CYCLIC INTERMED      89.1 MIL LB
N 000100425 STYRENE                                              FR
N 000100425
N 000100425                                                       CEH
N 000100425 STYRENE                                               SF
N 000100425 STYRENE                                             241ISO
N 000100425 MX8023629                                             MX
N 000100425 STYRENE                                               FA
E 000100425 0001
E 03 018783 021384 021995
```

Table 3-3 (continued)

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N 000100447  ALPHA-CHLOROTOLUENE (BENZYL CHLCRIDE)                80.4 MIL LBS  T72  CYCLIC INTERMED
N 000100447 BENZYL CHLORIDE                                         DC
N 000100447                                                         CEH
N 000100447 ALPHA-CHLOROTOLUENE                                   212ISO
N 000100447
E 000100447 0001
E 04 007887 008065 020119 021337

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N 000100516  BENZYL ALCOHCL                                       10.4 MIL LBS  T72  FLAVOR & PERFUME
N 000100516 BENZYL ALCOHOL                                          DC
N 000100516 BENZYL ALCOHOL                                          CT
N 000100516 BENZYL ALCOHOL                                        093GSO
N 000100516 MX8023947                                               MX
N 000100516 MX8023265                                               MX
N 000100516 MX8023594                                               MX
N 000100516 MX8023312                                               MX
N 000100516 MX8023163                                               MX
N 000100516 MX8024202                                               MX
N 000100516 BENZYL ALCOHOL                                          HA
N 000100516 MX8061947                                               MX
N 000100516 BENZYL ALCCHOL                                          FA
N 000100516 MX8052991                                               MX
N 000100516
N 000100516 BENZYL ALCOHCL                                          FC
N 000100516                                                         CEH
N 000100516 MX8017910                                               MX
N 000100516 MX8017547                                               MX
N 000100516 BENZYL ALCOHOL                                          SF
N 000100516 MX8026480                                               MX
N 000100516 MX8006766                                               MX
N 000100516 MX8006813                                               MX
N 000100516 MX8000348                                               MX
N 000100516 MX8000440                                               MX
N 000100516 MX8006686                                               MX
N 000100516 MX8000451                                               MX
N 000100516 BENZYL ALCOHOL                                          NP
N 000100516 MX8050519                                               MX
N 000100516 MX8049498                                               MX
N 000100516 MX8011527                                               MX
N 000100516 MX8012315                                               MX
E 000100516 0001
E 02 010843 021384

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N 000100527  BENZALDEHYDE, TECH.                                   4.6 MIL LBS  T72  CYCLIC INTERMED
N 000100527 MX8000417                                               MX
N 000100527 MX8006766                                               MX
N 000100527 MX8007805                                               MX
N 000100527 MX8006813                                               MX
N 000100527 MX8000440                                               MX
N 000100527 MX8014093                                               MX
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Table 3-3 (continued)

```
N 000100527 MX8030259                                                                          MX
N 000100527 MX8015961                                                                          MX
N 000100527 MX8030293                                                                          MX
N 000100527 MX8013761                                                                          MX
N 000100527 BENZALDEHYDE                                                                       SF
N 000100527                                                                                   CEH
N 000100527 BENZALDEHYDE                                                                       FC
N 000100527 MX8052220                                                                          MX
N 000100527 BENZALDEHYDE (BENZOIC ALDEHYDE)                                                    FA
N 000100527 MX8023947                                                                          MX
N 000100527 BENZALDEHYDE                                                                   091FSC
N 000100527 MX8023630                                                                          MX
N 000100527 BENZALDEHYDE                                                                        P
N 000100527 MX8027303                                                                          MX
N 000100527 BENZALDEHYDE                                                                       DC
N 000100527
E 000100527 0001
E 01 010843

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N 000100970  HEXAMETHYLENETETRAMINE                                                         95.2 MIL LBS  T72  MISC CHEMS                    60.4 MIL LB
N 000100970
N 000100970                                                                                   CEH
N 000100970 HEXAMETHYLENETETRAMINE                                                             DC
N 000100970 METHENAMINE                                                                        DC
N 000100970 HEXAMETHYLENETETRAMINE                                             1230        847704
N 000100970 MX8048871                                                                          MX
N 000100970 METHENAMINE                                                                        PD
N 000100970 HEXAMINE                                                                           AR
N 000100970 HEXAMETHYLENETETRAMINE                                                         107FSO
N 000100970 HEXAMETHYLENETETRAMINE                                                            FDA
N 000100970 HEXAMETHYLENETETRAMINE                                                            FDA
N 000100970 MX8047210                                                                          MX
N 000100970 MX8047232                                                                          MX
N 000100970 MX8047221                                                                          MX
N 000100970 MX8055627                                                                          MX
N 000100970 MX8022580                                                                          MX
E 000100970 0001
E 06 004585 005273 005274 007306 008633 011378

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N 000101213  ISOPROPYL N-(3-CHLOROPHENYL) CARBAMATE (CIPC)                                 2.0 MIL LBS  SRI  PESTICIDES
N 000101213                                                                                   CEH
N 000101213 MX8003358                                                                          MX
N 000101213 M-CHLOROCARBANILIC ACID, ISOPROPYL ESTER                                    382196
N 000101213
N 000101213 CIPC                                                                               FR
N 000101213 M-CHLOROCARBANILIC ACID, ISOPROPYL ESTER                                   253ESO
N 000101213 CHLOROPROPHAM (CHLORO-IPC)                                                          P
N 000101213 CIPC                                                                                P
E 000101213 0001
E 16 005869 007475 008911 008965 010779 010932 012942 013029 015238 016741 017426 017427 017848 018494 019528 020459

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Table 3-3 (continued)

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N 000102067  1,3-DIPHENYLGUANIDINE                                             5.0 MIL LBS  SRI  RUBBER-PROC CHEM
N 000102067 1,3-DIPHENYLGUANIDINE                                          429HSC
N 000102067
N 000102067                                                                   CEH
E 000102067 0001
E 02 011223 021757

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N 000102716  2,2',2"-NITRILOTRIETHANOL (TRIETHANOLAMINE)                     100.7 MIL LBS  T72  MISC CHEMS           35.8 MIL LB
N 000102716 TRIETHANOLAMINE                                                     CT
N 000102716 TRIETHANOLAMINE                                                     CT
N 000102716 TRIETHANCLAMINE                                                     CT
N 000102716 2,2',2''-NITRILOTRIETHANOL                                       31CSO
N 000102716 MX8054011                                                           MX
N 000102716 MX8059538                                                           MX
N 000102716 TRIETHANOLAMINE                                                     NP
N 000102716 TRIETHANOLAMINE                                                     DC
N 000102716 TRIETHANCLAMINE                                                     FC
N 000102716 MX8014151                                                           MX
N 000102716
E 000102716 0001
E 02 010843 013777

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N 000103231  DI(2-ETHYLHEXYL)ADIPATE                                           44.9 MIL LBS  T72  PLASTICIZERS         39.4 MIL LB
N 000103231                                                                   CEH
N 000103231
N 000103231 ADIPIC ACID, BIS(2-ETHYLHEXYL) ESTER DI(2-ETHYLHEXYL) ADIPATE   127ASO
N 000103231 DI-2-ETHYLHEXYL ADIPATE                                            FDA
N 000103231 DI(2-ETHYLHEXYL ADIPATE                                            FDA
N 000103231 DI(2-ETHYLHEXYL) ADIPATE                                           FDA
E 000103231 0001
E 01 020231

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N 000103695  N-ETHYLANILINE, REFINED                                            1.9 MIL LBS  T72  CYCLIC INTERMED
N 000103695                                                                   CEH
N 000103695
N 000103695 N-ETHYLANILINE                                                  223HSC
E 000103695 0001
E 01 005412

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N 000103844  ACETANILIDE, TECH.                                                 3.2 MIL LBS  T72  CYCLIC INTERMED
N 000103844                                                                   CEH
N 000103844 ACETANILIDE                                              211       167
N 000103844 ACETANILIDE                                                         NP
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Table 3-3 (continued)

```
N 000103844 MX8023334                                                    MX
N 000103844 ACETANILIDE                                              103GSO
N 000103844
N 000103844 ACETANILIDE                                                  DC
E 000103844 0001
E 05 006360 010349 010843 011166 021932

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N 000104552  CINNAMALDEHYDE                                             1.6 MIL LBS  T72  FLAVOR & PERFUME
N 000104552 MX8014093                                                    MX
N 000104552                                                             CEH
N 000104552 CINNAMALDEHYDE                                               SF
N 000104552 CINNAMALDEHYDE                                               FC
N 000104552 CINNAMIC ALDEHYDE                                            DC
N 000104552 CINNAMALDEHYDE                                               NP
N 000104552 MX8007805                                                    MX
N 000104552 MX8006799                                                    MX
N 000104552 MX8023630                                                    MX
N 000104552 MX8023947                                                    MX
N 000104552 CINNAMALDEHYDE                                           144DSO
N 000104552 CINNAMALDEHYDE (CINNAMIC ALDEHYDE)                           FA
N 000104552 MX8022728                                                    MX
N 000104552
E 000104552 0001
E 01 013451

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N 000106241  3,7-DIMETHYL-TRANS-2,6-OCTADIEN-1-OL (GERANIOL)            1.2 MIL LBS  T72  FLAVOR & PERFUME
N 000106241 GERANIOL                                                     CT
N 000106241                                                             CEH
N 000106241 GERANIOL                                                     DC
N 000106241 MX8000291                                                    MX
N 000106241 MX8008466                                                    MX
N 000106241 MX8007021                                                    MX
N 000106241 MX8006813                                                    MX
N 000106241 MX8000280                                                    MX
N 000106241 MX8008524                                                    MX
N 000106241 MX8000462                                                    MX
N 000106241 MX8008455                                                    MX
N 000106241 MX8007010                                                    MX
N 000106241 MX8006868                                                    MX
N 000106241 MX8016691                                                    MX
N 000106241 MX8016204                                                    MX
N 000106241 MX8014195                                                    MX
N 000106241 MX8016394                                                    MX
N 000106241 MX8014173                                                    MX
N 000106241 MX8027416                                                    MX
N 000106241 MX8014184                                                    MX
N 000106241 MX8050893                                                    MX
N 000106241 GERANIOL (3,7-DIMETHYL-2,6: 3,6-OCTADIEN-1-OL)               FA
N 000106241 MX8022795                                                    MX
N 000106241 MX8022740                                                    MX
N 000106241 3,7-DIMETHYL-TRANS-2,6-OCTADIEN-1-OL                     598DSC
N 000106241 MX8024133                                                    MX
N 000106241 MX8023243                                                    MX
```

Table 3-3 (continued)

```
N 000106241 MX8048519                                                             MX
N 000106241 MX8023925                                                             MX
N 000106241 MX8023594                                                             MX
N 000106241 MX8024257                                                             MX
N 000106241 MX8023652                                                             MX
N 000106241 MX8024122                                                             MX
N 00010624'
E 000106241 0001
E 01 010843

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N 000106467  P-DICHLOROBENZENE                                                  77.3 MIL LBS  T72  CYCLIC INTERMED      70.7 MIL LB
N 000106467
N 000106467 PARA-DICHLGROBENZENE                                                  DC
N 000106467                                                                      CEH
N 000106467 PARA-DICHLOROBENZENE                                         11485   CEH
N 000106467 P-DICHLOROBENZENE                                                     FR
N 000106467 P-DICHLORCBENZENE                                                     CT
N 000106467 PARADICHLOROBENZENE                                                   CT
N 000106467 DICHLOROBENZENE %PARA<                                                CT
N 000106467 PDB (PARA CICHLORO BENZENE)                                            P
N 000106467 P-DICHLOROBENZENE                                                 067HSO
E 000106467 0001
E 07 005170 005695 010789 010797 010810 012940 021600

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N 000106898  EPICHLORCHYDRIN                                                   354.0 MIL LBS  SRI  MISC CHEMS
N 000106898                                                                      CEH
N 000106898 EPICHLGHYDRIN                                                         FC
N 000106898 MX8000315                                                             MX
N 000106898 1-CHLORO-2,3-EPOXYPROPANE                                         157LSO
N 000106898 EPICHLCRCHYDRIN                                                       PR
N 000106898 EPICHLORCHYDRIN                                                       FA
N 000106898
E 000106898 0001
E 14 004641 005000 006982 009179 009212 009488 011454 012984 013640 016208 020626 021777 021912 021913

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N 000106934  1,2-DIBRCMOETHANE (ETHYLENE DIBRCHIDE)                            315.5 MIL LBS  T72  MISC CHEMS           304.4 MIL LB
N 000106934 1,2-DIBROMOETHANE                                                 149GSO
N 000106934 ETHYLENE CIBROMIDE                                                     P
N 000106934 ETHYLENE CIBROMIDE                                                     P
N 000106934 ETHYLENE UIBROMIDE                                                     P
N 000106934 MX8063705                                                             MX
N 000106934                                                                      CEH
N 000106934 MX8000224                                                             MX
N 000106934 MX8000246                                                             MX
N 000106934 MX8003074                                                             MX
N 000106934 ETHYLENE CICHLCRIDE                                                   FC
N 000106934
N 000106934 ETHYLENE CIBROMIDE                                                    CT
E 000106934 0002
```

Table 3-3 (continued)

```
E 18 004414 005480 006861 007225 007931 008212 011767 012223 012984 013608 014020 014101 015901 017636 017669 017827 018021 018022
E 12 018929 018937 019016 019337 020029 020037 020068 020762 021244 021245 021337 021925

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N 000106978  N-BUTANE                                                    2331.1 MIL LBS  T72  CRUDE PRODUCTS       23.3 MIL LB
N 000106978
N 000106978 BUTANE PRCPELLANT                                                CT
N 000106978 PROPELLENT %E.G. BUTANE<                                         CT
N 000106978 BUTANE                                                           PR
N 000106978 BUTANE                                                       083BSO
N 000106978 BUTANE                                                           FA
N 000106978 MX8006186                                                        MX
N 000106978 MX8006142                                                        MX
N 000106978 BUTANE                                                           FC
E 000106978 0001
E 03 011707 012699 012715

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N 000106989  1-BUTENE                                                      61.4 MIL LBS  T72  CRUDE PRODUCTS
N 000106989 1-BUTENE                                                     083CSO
N 000106989 AEROSOL PROPELENT %E.G. BUTENE<                                  CT
N 000106989
E 000106989 0001
E 03 011707 012699 012715

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N 000107062  1,2-DICHLCROETHANE (ETHYLENE DICHLORIDE)                    8600.0 MIL LBS  SRI  MISC CHEMS          540.2 MIL LB
N 000107062                                                                 CEH
N 000107062 MX8003063                                                        MX
N 000107062 ETHYLENE CICHLCPIDE                                              DC
N 000107062 MX8058773                                                        MX
N 000107062
N 000107062 ETHYLENE DICHLCPIDE                                               P
N 000107062 ETHYLENE CICHLORIDE                                             FDA
N 000107062 1,2-CICHLCROETHANE                                           079DSO
N 000107062 MX8063705                                                        MX
N 000107062 ETHYLENE CICHLORIDE                                              CT
E 000107062 0001
E 07 006699 009169 010780 019016 020029 020037 021347

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N 000107131  ACRYLCNITRILE                                               1114.7 MIL LBS  T72  MISC CHEMS           27.4 MIL LB
N 000107131
N 000107131                                                                 CEH
N 000107131 MX8002811                                                        MX
N 000107131 MX8013921                                                        MX
N 000107131 ACRYLCNITRILE                                                113DSO
N 000107131 ACRYLONITRILE                                                     P
N 000107131 ACRYLCNITPILE                                                   FDA
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Table 3-3 (continued)

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N 000107131 ACRYLONITRILE                                   FR
E 000107131 0001
E 04 004616 006618 008323 009488

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N 000107153  ETHYLENEDIAMINE                              59.4 MIL LBS  SRI  MISC CHEMS          22.5 MIL LB
N 000107153                                                CEH
N 000107153 MX8013409                                       MX
N 000107153 ETHYLENEDIAMINE                                 FC
N 000107153
N 000107153 ETHYLENEDIAMINE                             159JSO
E 000107153 0001
E 01 017366

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N 000107211  ETHYLENE GLYCOL                            3761.1 MIL LBS  T72  MISC CHEMS        2526.3 MIL LB
N 000107211 ETHYLENE GLYCOL                             160BSO
N 000107211 ETHYLENE GLYCOL                                FDA
N 000107211                                                CEH
N 000107211 ETHYLENE GLYCOL                                 DC
N 000107211 ETHYLENE GLYCOL                                KEM
N 000107211 MX8026935                                       MX
N 000107211 MX8012257                                       MX
N 000107211 GLYCOL                                          CT
N 000107211 ETHYLENE GLYCOL                                 CT
N 000107211
E 000107211 0001
E 11 006010 010798 011001 013043 013098 013911 016090 016515 019026 019340 021337

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N 000108010  2-DIMETHYLAMINOETHANOL                        3.5 MIL LBS  T72  MISC CHEMS
N 000108010 2-(DIMETHYLAMINO)ETHANOL                    065GSO
N 000108010                                                CEH
N 000108010
E 000108010 0001
E 01 005412

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N 000108054  VINYL ACETATE                              1210.7 MIL LBS  T72  MISC CHEMS          18.2 MIL LB
N 000108054 VINYL ACETATE                                   CT
N 000108054
N 000108054 VINYL ACETATE                               196BSO
N 000108054 VINYL ACETATE                                   FA
N 000108054 VINYL ACETATE                                   FC
N 000108054 MX8013987                                       MX
E 000108054 0001
E 01 021337
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Table 3-3 (continued)

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N 000108101  4-METHYL-2-PENTANONE (METHYL ISOBUTYL KETONE)           208.3 MIL LBS  T72  MISC CHEMS       201.0 MIL LB
N 000108101 4-METHYL-2-PENTANONE                                    278GSO
N 000108101 MX8048462                                                   MX
N 000108101 4-METHYL-2-PENTANONE                                        FA
N 000108101 METHYL ISO-BUTYL KETONE (4-METHYL-2-PENTANONE)              FA
N 000108101
N 000108101 METHYL ISOBUTYL KETONE                                      CT
N 000108101 METHYL ISOBUTYL KETONE                                      FR
N 000108101                                                            CEH
N 000108101 MX8003154                                                   MX
N 000108101 MX8030464                                                   MX
N 000108101 4-METHYL-2-PENTANONE                                        FC
N 000108101 METHYL ISOBUTYL KETONE                                      DC
N 000108101 4-METHYL-2-PENTANONE                                        SF
N 000108101 METHYL ISOBUTYL KETONE (MIBK)                              KEM
E 000108101 0001
E 01 004918

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N 000108203  ISOPROPYL ETHER                                          14.0 MIL LBS  SRI  MISC CHEMS        14.2 MIL LB
N 000108203 ISOPROPYL ETHER                                         273BSO
N 000108203
N 000108203 ISOPROPYL ETHER                                             CT
N 000108203                                                            CEH
N 000108203 ISOPROPYL ETHER                                             DC
E 000108203 0001
E 01 010843

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N 000108247  ACETIC ANHYDRIDE, 100%                                 1572.9 MIL LBS  T72  MISC CHEMS        39.4 MIL LB
N 000108247 ACETIC ANHYDRIDE                                        1170SC
N 000108247 ACETIC ANHYDRIDE                                            FA
N 000108247                                                            CEH
N 000108247 ACETIC ANHYDRIDE                                            FC
N 000108247
E 000108247 0001
E 01 014634

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N 000108781  MELAMINE                                                100.0 MIL LBS  SRI  CYCLIC INTERMED
N 000108781 MELAMINE                                                    PR
N 000108781 MELAMINE                                                   FDA
N 000108781 MELAMINE                                                    PR
N 000108781                                                            CEH
N 000108781 MELAMINE                                               299CSC
N 000108781
F 000108781 0001
E 02 010926 012771
```

Table 3-3 (continued)

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N 000108883  TOLUENE                                                   5917.2 MIL LBS  T72  CRUDE PRODUCTS      1074.2 MIL LB
N 000108883 TOLUENE                                                    190GSO
N 000108883 MX8023345                                                      MX
N 000108883                                                               CEH
N 000108883 TOLUENE                                                        DC
N 000109883 TOLUOL                                                        KEM
N 000108883 TOLUENE                                             369    421309
N 000108883 MX8007452                                                      MX
N 000108883 MX8011481                                                      MX
N 000108883 MX8017854                                                      MX
N 000108883 TOLUENE                                                        CT
N 000108883 AROMATICS, MONOCYCLIC %E.G. TOLUENE<                           CT
N 000108883 AROMATIC HYDROCARBONS SOLVENTS %E.G. TOLUENE<                  CT
N 000108883 AROMATIC HYDROCARBONS %E.G. TOLUENE<                           CT
N 000108883
N 000108883 TOLUENE                                                        CT
N 000108883 TOLUENE                                                        FR
E 000108883 0001
E 10 004630 007552 007729 010239 012940 014737 016468 018215 018904 021441

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N 000108907  CHLOROBENZENE, MONC                                        403.5 MIL LBS  T72  CYCLIC INTERMED
N 000108907                                                               CEH
N 000108907 MONOCHLOROBENZENE                                              CT
N 000108907 CHLOROBENZENE                                              208CSO
N 000108907 CHLOROBENZENE                                                 FDA
N 000108907
E 000108907 0001
E 03 004629 005098 005695

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N 000108941  CYCLOHEXANONE                                              784.4 MIL LBS  T72  CYCLIC INTERMED      51.0 MIL LB
N 000108941 CYCLOHEXANONE                                                21SO
N 000108941
N 000108941 CYCLOHEXANONE                                                  CT
N 000108941 CYCLOHEXANONE                                                  DC
N 000108941                                                               CEH
E 000108941 0001
E 03 004800 012318 014118

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N 000108952  PHENOL                                                    1915.5 MIL LBS  SRI  CYCLIC INTERMED      47.0 MIL LB
N 000108952                                                               CEH
N 000108952 CARBOLIC ACID                                                  NP
N 000108952 CARBOLIC ACID                                                  DC
N 000108952 PHENOL                                                         NP
N 000108952 MX8021916                                                      MX
N 000108952 MX8021827                                                      MX
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Table 3-3 (continued)

```
N 000108952 MX8003336                                             MX
N 000108952 MX8007452                                             MX
N 000108952 MX8002071                                             MX
N 000108952 MX8011481                                             MX
N 000108952 PHENOL                                            406292
N 000108952 PHENOL                                                DC
N 000108952 MX8027518                                             MX
N 000108952 MX8026957                                             MX
N 000108952 MX8027530                                             MX
N 000108952 MX8026719                                             MX
N 000108952 MX8013841                                             MX
N 000108952 MX8026568                                             MX
N 000108952 MX8027529                                             MX
N 000108952 MX8013692                                             MX
N 000108952 MX8012473                                             MX
N 000108952 MX8049432                                             MX
N 000108952 MX8050939                                             MX
N 000108952 MX8049374                                             MX
N 000108952 MX8049363                                             MX
N 000108952 MX8049501                                             MX
N 000108952 PHENOL                                                CT
N 000108952 CARBONIC ACID%PHENOL<                                 CT
N 000108952 PHENOL                                                FR
N 000108952 PHENOLS (E.G. PHENOL)                                 FR
N 000108952
N 000108952 MX8024600                                             MX
N 000108952 MX8024188                                             MX
N 000108952 MX8023356                                             MX
N 000108952 PHENOL                                           237CSO
N 000108952 PHENOL                                                PD
N 000108952 MX8054839                                             MX
N 000108952 MX8052173                                             MX
N 000108952 MX8050973                                             MX
N 000108952 MX8053927                                             MX
E 000108952 0001
E 15 004883 006911 006912 006983 009487 010651 010652 010817 010859 010947 011198 012940 020141 020657 020770

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N 000109739  MONO-N-BUTYLAMINE                                   4.0 MIL LBS  T72  MISC CHEMS
N 000109739
N 000109739                                                      CEH
N 000109739 BUTYLAMINE                                        134JSO
E 000109739 0001
E 01 004616

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N 000109897  DIETHYLAMINE                                       11.1 MIL LBS  T72  MISC CHEMS
N 000109897                                                      CEH
N 000109897 MX8014220                                             MX
N 000109897 DIETHYLAMINE                                      152BSO
N 000109897
E 000109897 0001
E 03 008791 015901 015918
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Table 3-3 (continued)

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N 000110054  TERT-BUTYL PEROXIDE (DI-TERT-BUTYL PEROXIDE)                    1.8 MIL LBS  T72  MISC CHEMS
N 000110054
N 000110054 TERT-BUTYL PEROXIDE                                           081HSC
N 000110054 TERT-BUTYL PEROXIDE                                              FDA
N 000110054                                                                  CEH
E 000110054 0001
E 01 017841

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N 000110178  FUMARIC ACID                                                   51.5 MIL LBS  T72  MISC CHEMS          16.2 MIL LB
N 000110178 FUMARIC ACID                                                      CT
N 000110178 FUMARIC ACID                                                  613CSD
N 000110178 FUMARIC ACID                                                      FA
N 000110178                                                                  CEH
N 000110178 FUMARIC ACID                                                      SF
N 000110178 FUMARIC ACID (ROSIN ADDUCT, ESTERIFIED WITH GLYCERIN)             FC
N 000110178 FUMARIC ACID                                                      FC
N 000110178 FUMARIC ACID                                                      FC
N 000110178 FUMARIC ACID                                                      DC
N 000110178
E 000110178 0001
E 03 005412 009270 019499

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N 000110441  SORBIC ACID                                                    40.0 MIL LBS  SRI  MISC CHEMS          20.6 MIL LB
N 000110441 MX8048268                                                         MX
N 000110441 SORBIC ACID                                                   286BSD
N 000110441 MX8056448                                                         MX
N 000110441 SORBIC ACID                                                       FA
N 000110441 SORBIC ACID                                                       DC
N 000110441 SORBIC ACID                                                       FC
N 000110441 SORBIC ACID                                                  147
N 000110441                                                                  CEH
N 000110441 MX8050451                                                         MX
N 000110441
E 000110441 0001
E 02 009270 021296

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N 000110805  ETHYLENE GLYCOL MONOETHYL ETHER (2-ETHOXYETHANOL)             205.4 MIL LBS  T72  MISC CHEMS         197.5 MIL LB
N 000110805 CELLOSOLVE %ETHYLENE GLYCOL MONOETHYL ETHER<                      CT
N 000110805 MONOETHYL ETHERS OF ETHYLENE GLYCOL                               CT
N 000110805                                                                  CEH
N 000110805
N 000110805 2-ETHOXYETHANOL                                              158ISC
E 000110805 0001
E 01 005412
```

Table 3-3 (continued)

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N 000110827  CYCLOHEXANE                       2298.4 MIL LBS  T72  CYCLIC INTERMED      94.2 MIL LB
N 000110827                                       CEH
N 000110827 CYCLOHEXANE                        215CSO
N 000110827
N 000110827 CYCLCHEXANE                            CT
E 000110827 0001
E 03 004629 004630 021337

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N 000110850  PIPERAZINE                           3.6 MIL LBS  T72  MEDICINAL CHEMS
N 000110850 MX8017901                              MX
N 000110850                                       CEH
N 000110850 PIPERAZINE                             DC
N 000110850 MX8026822                              MX
N 000110850 MX8028862                              MX
N 000110850 MX8027756                              MX
N 000110850 MX8026888                              MX
N 000110850 MX8027814                              MX
N 000110850 MX8026866                              MX
N 000110850 MX8026855                              MX
N 000110850 MX8026844                              MX
N 000110850 PIPERAZINE BASE                        CT
N 000110850
N 000110850 MX8047276                              MX
N 000110850 PIPERAZINE                         036ASO
N 000110850 MX8057145                              MX
N 000110850 MX8056631                              MX
E 000110850 0001
E 04 005412 013479 014037 016299

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N 000110918  MORPHOLINE                          23.3 MIL LBS  T72  MISC CHEMS           12.4 MIL LB
N 000110918
N 000110918 MORPHOLINE                             CT
N 000110918 MORPHOLINE                             CT
N 000110918 MORPHOLINE                         279ASO
N 000110918 MORPHOLINE                          751
N 000110918                                       CEH
N 000110918 MORPHOLINE                             FC
N 000110918 MORPHOLINE                            KEM
E 000110918 0001
E 06 008594 014037 014995 016299 017876 018448

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N 000111400  DIETHYLENETRIAMINE                  32.4 MIL LBS  T72  MISC CHEMS           16.7 MIL LB
N 000111400 DIETHYLENETRIAMINE                 152JSO
N 000111400 DIETHYLENETRIAMINE                    FDA
N 000111400 2,2-DIAMINODIETHYLAMINE                CT
N 000111400
```

Table 3-3 (continued)

```
N 000111400                                                       CEH
E 000111400 0001
E 02 004616 005412

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N 000111422  2,2'-IMINODIETHANOL (DIETHANOLAMINE)              101.1 MIL LBS  T72  MISC CHEMS        36.0 MIL LB
N 000111422 DIETHANOLAMINE                                       FDA
N 000111422 2,2'-IMINODIETHANOL                                061DSO
N 000111422 DIETHANOLAMINE                                        CT
N 000111422 DIETHANOLAMINE                                        CT
N 000111422                                                      CEH
N 000111422 DIETHANOLAMINE                                        DC
N 000111422 DIETHANOLAMINE                                        DC
N 000111422
E 000111422 0001
E 03 011454 016019 019324

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N 000111922  DI-N-BUTYLAMINE                                     3.8 MIL LBS  T72  MISC CHEMS
N 000111922
N 000111922 DIBUTYLAMINE                                       255HSO
N 000111922                                                      CEH
E 000111922 0001
E 01 005412

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N 000112276  TRIETHYLENE GLYCOL MONOETHYL ETHER                 21.2 MIL LBS  T72  MISC CHEMS        21.5 MIL LB
N 000112276 TRIETHYLENE GLYCOL                                    CT
N 000112276 TRIETHYLENEGLYCOLS                                    FR
N 000112276
N 000112276                                                      CEH
N 000112276 TRIETHYLENE GLYCOL                                    DC
N 000112276 TRIETHYLENE GLYCOL                                 193JSO
E 000112276 0001
E 01 019026

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N 000115071  PROPYLENE                                        8471.6 MIL LBS  T72  CRUDE PRODUCTS    127.1 MIL LB
N 000115071                                                      CEH
N 000115071
N 000115071 PROPANE                                            184LSO
E 000115071 0001
E 01 012699

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N 000115297  ENDOSULFAN                                          2.0 MIL LBS  SRI  PESTICIDES
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Table 3-3 (continued)

```
N 000115297 1,4,5,6,7,7-HEXACHLORO-5-NORBORNENE-2,3-DIMETHANOL, CYCLIC SULFI543HSO
N 0001152971TE                                                         543HSO
N 000115297
N 000115297 THIODAN (ENDOSULFAN)                                            P
N 000115297 ENDOSULFAN                                                      P
E 000115297 0001
E 03 013239 016741 020762

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N 000115322  4,4'-DICHLORO-ALPHA-TRICHLOROMETHYLBENZHYDROL (DICOFOL)           4.0 MIL LBS  SRI  PESTICIDES
N 000115322                                                                  CEH
N 000115322
N 000115322 4,4'-DICHLORO-ALPHA-(TRICHLOROMETHYL)BENZHYDROL                256JSC
N 000115322 KELTHANE (DICOFOL)                                                  P
N 000115322 KELTHANE                                                            P
N 000115322 DICOFOL                                                             P
E 000115322 0001
E 05 013248 014190 016741 021385 022827

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N 000115866  TRIPHENYL PHOSPHATE                                               10.6 MIL LBS  T70  PLASTICIZERS
N 000115866 TRIPHENYL PHOSPHATE                                            181GSO
N 000115866 TRIPHENYL PHOSPHATE                                                AR
N 000115866 TRIPHENYLPHOSPHATE                                                FDA
N 000115866
N 000115866                                                                   CEH
E 000115866 0001
E 01 005412

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N 000117817  DI(2-ETHYLHEXYL)PHTHALATE                                        435.0 MIL LBS  T72  PLASTICIZERS        441.6 MIL LB
N 000117817 DI(2-ETHYLHEXYL) PHTHALATE                                        FDA
N 000117817 DI(2-ETHYLHEXYL) PHTHALATE                                        FDA
N 000117817 PHTHALIC ACID, BIS(2-ETHYLHEXYL) ESTER                         183CSO
N 000117817                                                                   CEH
N 000117817
E 000117817 0001
E 03 010172 017788 020167

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N 000119368  METHYL SALICYLATE                                                  5.8 MIL LBS  T72  FLAVOR & PERFUME
N 000119368 SALICYLIC ACID, METHYL ESTER                                   137ESO
N 000119368 METHYL SALICYLATE                                                  FA
N 000119368 MX8048371                                                          MX
N 000119368 MX8023356                                                          MX
N 000119368 MX8024542                                                          MX
N 000119368 008060502                                                          MX
N 000119368 MX8058319                                                          MX
N 000119368 MX8051012                                                          MX
```

Table 3-3 (continued)

```
N 000119368 MX8052775
N 000119368 MX8022964                                            MX
N 000119368                                                      MX
N 000119368 METHYL SALICYLATE                                   CEH
N 000119368 MX8006813                                            FC
N 000119368 MX8000348                                            MX
N 000119368 METHYL SALICYLATE                                    MX
N 000119368 METHYL SALICYLATE                                    SF
N 000119368 METHYL SALICYLATE                                    DC
N 000119368 SWEET BIRCH OIL                                      NP
N 000119368 MX8030839                                            NP
N 000119368 MX8026957                                            MX
N 000119368 MX8017116                                            MX
N 000119368 METHYL SALICYLATE                                    MX
N 000119368 UIL OF WINTERGREEN %METHYL SALICYLATE<               CT
N 000119368                                                      CT
E 000119368 0001
E 02 005921 009617

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N 000121335  VANILLIN, SYNTHETIC
N 000121335                                                      4.0 MIL LBS  SRI  FLAVOR & PERFUME
N 000121335 VANILLA
N 000121335 VANILLIN                                             NF
N 000121335 MX8013567                                            CT
N 000121335 VANILLIN                                             MX
N 000121335 VANILLA                                              NP
N 000121335 VANILLIN                                             DC
N 000121335 VANILLA                                              SF
N 000121335 VANILLIN                                             FC
N 000121335                                                      FC
N 000121335 MX8048882                                           CEH
N 000121335 MX8048984                                            MX
N 000121335 MX8030293                                            MX
N 000121335 MX8014424                                            MX
N 000121335 MX8026902                                            MX
N 000121335 MX8007009                                            MX
N 000121335 MX8011890                                            MX
N 000121335 MX8007065                                            MX
N 000121335 MX8000348                                            MX
N 000121335 MX8023607                                            MX
N 000121335 MX8024235                                            MX
N 000121335 MX8047312                                            MX
N 000121335 MX8023629                                            MX
N 000121335 MX8022820                                            MX
N 000121335 MX8052220                                            MX
N 000121335 VANILLIN                                             MX
N 000121335 VANILLA (VANILLIN)                               289ESO
E 000121335 0001                                                 FA
E 02 005412 020784

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N 000121755  MALATHION
N 000121755                                                      30.0 MIL LBS  SRI  PESTICIDES        30.3 MIL LB
N 000121755 MX8026366                                            CEH
                                                                 MX
```

Table 3-3 (continued)

```
N 000121755
N 000121755 MALATHION                                                         CT
N 0001217551PHOSPHORODITHIOATE                                             274BSO
N 000121755 MERCAPTOSUCCINIC ACID, DIETHYL ESTER, S-ESTER WITH O,O-DIMETHYL 274BSO
N 000121755 O,O-DIMETHYL DITHIOPHOSPHATE OF DIETHYL MERCAPTOSUCCINATE           P
N 000121755 MALATHION                                                           P
E 000121755 0001
E 18 012999 013248 014190 014443 014546 016163 016302 016741 017984 020762 021337 021385 021799 021918 021928 022827 022877 022878

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N 000122349  2-CHLORO-4,6-BIS(ETHYLAMINO)-S-TRIAZINE (SIMAZINE)          5.0 MIL LBS  SRI  PESTICIDES
N 000122349
N 000122349 2-CHLORO-4,6-BIS(ETHYLAMINO)-S-TRIAZINE                  559CSC
N 000122349 SIMAZINE                                                      P
N 000122349 SIMAZINE                                                      P
N 000122349 MX8000520                                                    MX
N 000122349 2-CHLORO-4,6-BIS(ETHYLAMINO)-S-TRIAZINE                    626
N 000122349                                                             CEH
E 000122349 0001
E 18 005094 005230 005591 006618 008309 009537 010771 010772 011281 013029 017078 019263 020762 021083 021385 022812 022827 022878

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N 000122394  DIPHENYLAMINE                                               33.8 MIL LBS  T72  CYCLIC INTERMED
N 000122394
N 000122394                                                             CEH
N 000122394 DIPHENYLAMINE                                            222FSC
N 000122394 DIPHENYLAMINE                                                 P
N 000122394 DIPHENYLAMINE                                                 P
N 000122394 DIPHENYLAMINE                                                CT
E 000122394 0001
E 01 015918

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N 000123319  HYDROQUINONE, TECH.                                         11.8 MIL LBS  T72  CYCLIC INTERMED
N 000123319                                                             CEH
N 000123319 MX8046671                                                    MX
N 000123319 MX8027029                                                    MX
N 000123319 MX8028588                                                    MX
N 000123319 MX8048597                                                    MX
N 000123319 HYDROQUINONE                                                 CT
N 000123319 HYDROQUINONE                                             225DSO
N 000123319 HYDROQUINONE                                                 PD
N 000123319
E 000123319 0001
E 17 004616 006192 009488 009584 010651 010652 010936 011162 011275 012235 012602 012940 014375 014542 016576 017242 021260

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N 000123331  1,2-DIHYDROPYRIDAZINE-3,6-DIONE (MALEIC HYDRAZIDE)          4.5 MIL LBS  T72  PESTICIDES
N 000123331
```

Table 3-3 (continued)

```
N 000123331 1,2-DIHYDRO-3,6-PYRIDAZINEDIONE                                 257LSD
N 000123331 MALEIC HYDRAZIDE (MH-30)                                             P
N 000123331                                                                    CEH
N 000123331 1,2-DIHYDRO-3,6-PYRIDAZINEDIONE                                889654
E 000123331 0006
E 18 004466 004492 004567 004640 004906 004908 004909 004910 004911 005043 005230 005254 005412 005532 005567 005568 005591 005871
E 18 006036 006379 006449 006478 006496 006553 006629 006806 006820 006942 006957 007117 007463 007566 007732 008323 009202 010661
E 18 010699 010704 010724 010740 010773 010774 010775 010794 010835 010860 010870 010905 010953 011012 011267 011638 011694 011714
E 18 011756 011762 011788 011819 012169 012240 012701 012790 012797 012978 012979 012984 013017 013029 013039 013954 014033 014182
E 18 014860 015109 015420 015441 016078 016122 016156 016216 016496 016631 016716 017012 017014 017412 018878 019264 020094 020572
E 12 020749 020800 020941 021272 021322 021337 021420 021468 021481 021696 022417 022850

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N 000123911  DIOXANE                                                          13.8 MIL LBS  T72  MISC CHEMS            14.0 MIL LB
N 000123911 DIOXANE                                                             CT
N 000123911
N 000123911 P-DIOXANE                                                       068DSC
N 000123911                                                                    CEH
E 000123911 0001
E 05 006917 010843 014210 016090 019071

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N 000124287  N,N-DIMETHYLOCTADECYLAMINE                                        1.5 MIL LBS  T72  SURF-ACTIV AGENT
N 000124287
N 000124287 N,N-DIMETHYLOCTADECYLAMINE                                      453BSC
N 000124287  N,N-DIMETHYLOCTADECYLAMINE                                        1.5 MIL LBS  SRI  SURF-ACTIV AGENT
E 000124287 0001
E 01 005412

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N 000124403  DIMETHYLAMINE                                                    95.9 MIL LBS  T72  MISC CHEMS            20.6 MIL LB
N 000124403 DIMETHYLAMINE                                                   155CSC
N 000124403
E 000124403 0001
E 07 005412 008791 009525 011168 011789 014523 020059

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N 000127093  SODIUM ACETATE                                                   18.1 MIL LBS  T71  MISC CHEMS
N 000127093
N 000127093 SODIUM ACETATE                                                      HA
N 000127093 SODIUM ACETATE                                                      FA
N 000127093 MX8053369                                                           MX
N 000127093 SODIUM ACETATE                                                      DC
N 000127093 SODIUM ACETATE                                                      FC
N 000127093 SODIUM ACETATE                                                      FC
N 000127093 MX8002888                                                           MX
N 000127093 MX8002899                                                           MX
N 000127093 MX8002866                                                           MX
N 000127093                                                                    CEH
```

Table 3-3 (continued)

```
N 000127093 MX8027529                                                  MX
N 000127093 MX8027530                                                  MX
N 000127093 MX9027513                                                  MX
N 000127093 MX8027041                                                  MX
N 000127093 SODIUM ACETATE                                             NP
N 000127093 MX8013337                                                  MX
N 000127093 MX8049498                                                  MX
N 000127093 SODIUM ACETATE                                             CT
F 000127093 0001
F 05 004956 012672 013636 018012 020671

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N 000127184  TETRACHLOROETHYLENE (PERCHLOROETHYLENE)                734.2 MIL LBS  T72  MISC CHEMS        588.0 MIL LB
N 000127184
N 000127184 TETRACHLOROETHYLENE                                   125SC
N 000127184 PERCHLOROETHYLENE                                        DC
N 000127184                                                         CEH
N 000127184 TETRACHLOROETHYLENE                                      NP
N 000127184 PERCHLORETHYLENE                                         CT
N 000127184 PERCHLORETHYLENE                                         CT
N 000127184 PERCHLOROETHYLENE                                        CT
N 000127184 PERCHLOROETHYLENE                                        FR
N 000127184 PERCHLOROETHYLENE                                        FR
E 000127184 0001
E 01 021339

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N 000127208  2,2-DICHLOROPROPIONIC ACID, SODIUM SALT (DALAPON)       5.0 MIL LBS  SRI  PESTICIDES
N 000127208 2,2-DICHLOROPROPIONIC ACID SODIUM SALT                065FSC
N 000127208 DALAPON                                                   P
N 000127208 DALAPON                                                   P
N 000127208                                                         CEH
N 000127208
F 000127208 0001
F 01 019262

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N 000128041  DIMETHYLDITHIOCARBAMIC ACID, SODIUM SALT                4.6 MIL LBS  T72  RUBBER PROC CHEMS
N 000128041 DIMETHYLDITHIOCARBAMIC ACID SODIUM SALT               259DSC
N 000128041 DIBAM (SODIUM DIMETHYL DITHIOCARBAMATE)                   P
N 000128041
N 000128041                                                         CEH
N 000128041 MX8000962                                                MX
E 000128041 0001
E 01 013176

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N 000128370  2,6-DI-TERT-BUTYL-P-CRESOL                              7.5 MIL LBS  T72  MISC CHEMS
N 000128370 2,6-DI-TERT-BUTYL-P-CRESOL                            163ASO
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Table 3-3 (continued)

```
N 000128370 MX8047356                                                        MX
N 000128370 BHT                                                              FA
N 000128370 BUTYLATED HYDROXYTOLUENE (BHT)                                   FA
N 000128370 BUTYLATED HYDROXYTOLUENE                                         FA
N 000128370
N 000128370 2,6-DI-TERT-BUTYL-P-CRESOL                                     209
N 000128370                                                                 CEH
N 000128370 BUTYLATED HYDROXYTOLUENE (DI-TERTIARY-BUTYL-PARA-CRESOL) (2,6-DI-   FC
N 000128370 TERTIARY-BUTYL-4-METHYL PHENOL)                                  FC
N 000128370  2,6-DI-TERT-BUTYL-P-CRESOL, TECH.                           17.8 MIL LBS  T72  MISC CHEMS          18.4 MIL LB
F 000128370 0001
E 10 005004 005412 011163 014858 016076 017284 019646 020850 020877 020887

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N 000129679  ENDOTHALL                                                    2.0 MIL LBS  SRI  PESTICIDES
N 000129679 ENTOTHALL                                                        P
N 000129679 ENDOTHALL                                                        P
N 000129679 7-OXABICYCLO(2.2.1)HEPTANE-2,3-DICARBOXYLIC ACID DISODIUM SALT  177LSO
N 000129679
N 000129679                                                                 CEH
F 000129679 0001
E 02 012109 013029

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N 000133062  N-TRICHLOROMETHYLTHIO-4-CYCLOHEXENE-1,2-DICARBOXIMIDE (CAPTAN)   18.0 MIL LBS  SRI  PESTICIDES          18.2 MIL LB
N 000133062 CAPTAN                                                           P
N 000133062 N-TRICHLOROMETHYLTHIO-4-CYCLOHEXENE-1,2-DICARBOXIMIDE            P
N 000133062 N-((TRICHLOROMETHYL)THIO)-4-CYCLOHEXENE-1,2-DICARBOXIMIDE      356ISO
N 000133062
N 000133062 MX8059918                                                        MX
N 000133062                                                                 CEH
N 000133062 MX8012406                                                        MX
N 000133062IDE
N 000133062 N-((TRICHLOROMETHYL)THIO)-4-CYCLOHEXENE-1,2-DICARBOXIMI        798
N 000133062 N-TRICHLOROMETHYLMERCAPTO 4-CYCLOHEZENE-1,2 DICARBOXIMIDE        NP
E 000133062 0003
E 18 005412 005720 005896 007226 007231 007233 007234 007717 007845 008833 009117 012813 012976 012984 013248 013249 013293 013317
F 18 013608 014101 015108 015225 015579 015702 015703 016738 017214 017666 018426 018619 018858 020061 020119 020264 020691 020762
E 14 020856 021337 021362 021385 021799 022096 022301 022328 022331 022338 022818 022827 022877 022878

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N 000133073  N-TRICHLOROMETHYLTHIOPHTHALIMIDE (FOLPET)                     2.0 MIL LBS  SRI  PESTICIDES
N 000133073 N-((TRICHLOROMETHYL)THIO)PHTHALIMIDE                          799
N 000133073                                                                CEH
N 000133073
N 000133073 N-((TRICHLOROMETHYL)THIO)PHTHALIMIDE                        366HSO
N 000133073 FOLPET                                                          P
N 000133073 PHALTAN (N-(TRICHLOROMETHYLTHIO) PHTHALIMIDE)                   P
N 000133073 FOLPET (PHALTAN)                                                P
E 000133073 0001
E 16 007717 012814 015225 015703 017536 017899 020061 020264 020762 021337 021395 021799 021958 022827 022877 022878
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Table 3-3 (continued)

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N 000133904  2,5-DICHLORO-3-AMINOBENZOIC ACID, AMMONIUM SALT (AMIBEN)           20.0 MIL LBS  SRI  PESTICIDES        20.2 MIL LB
N 000133904                                                                       CEH
N 000133904
N 000133904 3-AMINO-2,5-DICHLOROBENZOIC ACID                                    304CSC
N 000133904 AMIBEN                                                                  M
N 000133904 AMIBEN                                                                  P
E 000133904 0001
E 02 012433 013029

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N 000134623  N,N-DIETHYLTOLUAMIDE (DEET)                                           1.0 MIL LBS  SRI  PESTICIDES
N 000134623 DIETHYL TOLUAMIDE (DEET)                                                P
N 000134623 N,N-DIETHYL-M-TOLUAMIDE                                             048DSC
N 000134623                                                                       CEH
N 000134623
N 000134623 N-N'-DIETHYL TOLUAMIDE                                                 CT
E 000134623 0001
E 01 013248

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N 000137268  BIS(DIMETHYLTHIOCARBAMOYL) DISULFIDE                                 13.1 MIL LBS  T72  RUBBER PROC CHEMS
N 000137268 THIRAM (ARASAN)                                                         P
N 000137268 THIRAM                                                                FDA
N 000137268 BIS(DIMETHYLTHIOCARBAMOYL)DISULFIDE                                  298SC
N 000137268 TETRAMETHYLTHIURAM DISULPHIDE                                           C
N 000137268                                                                       CEH
N 000137268 BIS(DIMETHYLTHIOCARBAMYL) DISULFIDE                                   KEM
N 000137268 MX8005456                                                              MX
N 000137268 TRIPALMITIN                                               205        163
E 000137268 0001
E 14 008085 012316 012316 015108 017214 017423 018843 019513 020691 021385 021606 021799 022329 022480

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N 000137304  DIMETHYLDITHIOCARBAMIC ACID                                           2.4 MIL LBS  T72  RUBBER PROC CHEMS
N 000137304
N 000137304 DIMETHYLDITHIOCARBAMIC ACID ZINC SALT                               259ESC
N 000137304 ZIRAM (ZINC DIMETHYL DITHIOCARBAMATE)                                   P
N 000137304 MX8053154                                                              MX
N 000137304 MX8003427                                                              MX
N 000137304 BIS(DIMETHYLDITHIOCARBAMATO)ZINC                                      52
N 000137304 MX8059743                                                              MX
N 000137304 ZINC DIMETHYLDITHIOCARBAMATE                                           CT
E 000137304 0001
E 13 006619 007717 007949 008085 010968 012481 012482 017423 020691 020752 021385 022480 022827

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Table 3-3 (continued)

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N 000137406  SODIUM PROPIONATE                                                  4.1 MIL LBS  T72  MISC CHEMS
N 000137406
N 000137406 PROPIONIC ACID SODIUM SALT                                      283GSC
N 000137406 MX8055398                                                           MX
N 000137406 MX8055401                                                           MX
N 000137406 MX8056313                                                           MX
N 000137406 MX8024666                                                           MX
N 000137406 MX8025487                                                           MX
N 000137406 SODIUM PROPIONATE                                                   FA
N 000137406                                                                    CEH
N 000137406 MX8059594                                                           MX
N 000137406 SODIUM PRCPIONATE                                                   NP
N 000137406 SODIUM PRCPIONATE                                                   FC
N 000137406 MX8014582                                                           MX
N 000137406 MX8014571                                                           MX
N 000137406 MX8027085                                                           MX
N 000137406 SODIUM PROPIONATE                                                   CT
E 000137406 0001
E 01 011645

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N 000141435  2-AMINCETHANOL (MONCETHANOLAMINE)                                 82.1 MIL LBS  T72  MISC CHEMS          29.3 MIL LB
N 000141435
N 000141435 MONOETHANCLAMINE                                                    CT
N 000141435 ETHANOLAMINE                                                        CT
N 000141435 2-AMINOETHANOL                                                  1271SC
N 000141435 MONOETHANCLAMINE                                                    DC
N 000141435 MX8030328                                                           MX
N 000141435 MX8030339                                                           MX
E 000141435 0001
E 05 010843 011454 015324 019343 022088

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N 000141537  SODIUM FORMATE, TECH.                                             32.0 MIL LBS  SRI  MISC CHEMS          22.9 MIL LB
N 000141537 FORMIC ACID SODIUM SALT                                         1620SC
N 000141537 SODIUM FORMATE                                                     FDA
N 000141537                                                                    CEH
N 000141537 MX9048633                                                           MX
N 000141537
E 000141537 0001
E 01 011162

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N 000142472  MONOSODIUM GLUTAMATE                                              47.3 MIL LBS  T72  FLAVOR & PERFUME    51.4 MIL LB
N 000142472                                                                    CEH
N 000142472 GLUTANIC ACID SALTS (E.G. MONOSODIUM GLUTAMATE)                     DC
N 000142472 MONOSODIUM GLUTAMATE                                                FC
N 000142472 MX8027530                                                           MX
N 000142472 MX8027518                                                           MX
N 000142472 MX8027529                                                           MX
N 000142472
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Table 3-3 (continued)

```
N 000142472 GLUTAMIC ACID SODIUM SALT                           118CSC
N 000142472 MONOSODIUM GLUTAMATE                                    FA
N 000142472 MX8060580                                               MX
N 000142472 MX8053016                                               MX
E 000142472 0001
E 04 014085 019481 020784 020900

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N 000143077  LAURIC ACID                                        2.0 MIL LBS  T72  SURF-ACTIV AGENT
N 000143077 LAURIC ACID                                         467CSC
N 000143077 LAURIC ACID                                             FP
N 000143077 MX8027303                                               MX
N 000143077 DODECANOIC ACID (LAURIC ACID)                           FA
N 000143077 LAURIC ACID                                             FA
N 000143077 MX8048042                                               MX
N 000143077 MX8047743                                               MX
N 000143077 MX8023390                                               MX
N 000143077 MX8023050                                               MX
N 000143077                                                        CEH
N 000143077 LAURIC ACID                                             DC
N 000143077 MX8013272                                               MX
N 000143077 LAURIC ACID                                             NP
N 000143077 LAURIC ACID                                             FC
N 000143077 MX8014593                                               MX
N 000143077 MX8014491                                               MX
N 000143077 MX8014479                                               MX
N 000143077 MX8000622                                               MX
N 000143077
E 000143077 0001
E 01 012992

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N 000149304  2-MERCAPTOBENZOTHIAZOLE                            6.0 MIL LBS  T72  RUBBER PROC CHEMS
N 000149304
N 000149304 MERCAPTOBENZENE THIAZOLE %CORROSION INHIBITOR<          CT
N 000149304 MERCAPTOBENZOTHIAZOLE                                   CT
N 000149304                                                        CEH
N 000149304 MX8003449                                               MX
N 000149304 2-BENZOTHIAZOLETHIOL                                156NSC
N 000149304 MX8053154                                               MX
E 000149304 0001
E 01 005412

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N 000151213  2-ETHYLHEXYL SULFATE, SODIUM SALT                 10.0 MIL LBS  SRI  SURF-ACTIV AGENT
N 000151213 SODIUM LAURYL SULFATE                                   FA
N 000151213 MX8023403                                               MX
N 000151213 MX8022615                                               MX
N 000151213 MX8023035                                               MX
N 000151213
N 000151213 SODIUM LAURYL SULFATE                                   CT
N 000151213 DODECYL SULFATE SODIUM SALT                         371ISC
```

Table 3-3 (continued)

```
N 000151213 N-DODECYL SULFATE, SODIUM SALT                     14463  CEH
N 000151213 MX8050633                                                  MX
N 000151213 MX8012564                                                  MX
N 000151213 MX8049523                                                  MX
N 000151213 MX8048564                                                  MX
N 000151213 SODIUM LAURYL SULFATE                                      DC
N 000151213 SODIUM LAURYL SULFATE                                      NP
N 000151213 MX8014388                                                  MX
N 000151213 IRIUM                                                      NP
N 000151213 ALKYL SULFATE                                              NP
N 000151213 MX8012100                                                  MX
N 000151213 MX8028599                                                  MX
N 000151213 SODIUM LAURYL SULFATE                                      FC
N 000151213 MX8059765                                                  MX
N 000151213 MX8059390                                                  MX
N 000151213  DODECYL SULFATE, SODIUM SALT                           26.8 MIL LBS  T72  SURF-ACTIV AGENT     27.6 MIL LB
E 000151213 0001
E 11 004889 006126 008026 010102 010817 014965 015359 016277 019336 021754 022431

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N 000298000  PHOSPHOROTHIOATE (METHYL PARATHION)                     51.1 MIL LBS  T72  PESTICIDES           52.7 MIL LB
N 000298000 PHOSPHOROTHIOIC ACID, O,O-DIMETHYL O-P-NITROPHENYL ESTER  315HSC
N 000298000
N 000298000 METHYL PARATHION (METACIDE                                  P
N 000298000 MX8003983                                                  MX
E 000298000 0001
E 11 007094 014443 014546 016163 016741 017984 020762 021918 021929 022877 022878

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N 000298022  O,O-DIETHYL S-(ETHYLTHIO)METHYL PHOSPHORODITHIOATE (PHORATE)      8.0 MIL LBS  SRI  PESTICIDES
N 000298022
N 000298022 PHOSPHORODITHIOIC ACID, O,O-DIETHYL S-((ETHYLTHIO)METHYL) ESTER 232ESO
N 000298022 THIMET                                                      P
N 000298022 PHORATE                                                     P
N 000298022                                                            CEH
E 000298022 0001
E 02 022877 022878

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N 000298044  DISULFOTON                                               8.0 MIL LBS  SRI  PESTICIDES
N 000298044
N 000298044 PHOSPHORODITHIOIC ACID, O,O-DIETHYL S-(2-(ETHYLTHIO)ETHYL) ESTER315FSO
N 000298044 DI-SYSTON (DISULFOTON)                                      P
N 000298044                                                            CEH
E 000298044 0001
E 02 014546 020176

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N 000300765  1,2-DIBROMO-2,2-DICHLOROETHYL DIMETHYL PHOSPHATE (NALED)          2.0 MIL LBS  SRI  PESTICIDES
```

Table 3-3 (continued)

```
N 000300765 NALED                                                                 P
N 000300765 NALED (DIBROM)                                                        P
N 000300765 DIBROM (1,2-DIBROMO-2, 2-DICHLOROETHYL DIMETHYL PHOSPHATE)            P
N 000300765 PHOSPHORIC ACID, 1,2-DIBROMO-2,2-DICHLOROETHYL DIMETHYL ESTER    337HSO
N 000300765
N 000300765                                                                     CEH
F 000300765 0001
E 02 016741 020176

----------------------------------------------------------------------------------------------------------------------------

N 000309002  ALDRIN                                                             25.0 MIL LBS  SRI  PESTICIDES         25.3 MIL LB
N 000309002 ALDRIN                                                               CT
N 000309002                                                                     CEH
N 000309002
N 000309002 ALDRIN                                                                P
E 000309002 0001
E 11 006618 008197 005044 009124 010806 012984 014190 020048 020762 021385 022827

----------------------------------------------------------------------------------------------------------------------------

N 000314409  5-BROMO-3-SEC-BUTYL-6-METHYLURACIL (BROMACIL)                        8.0 MIL LBS  SRI  PESTICIDES
N 000314409 MX8012586                                                            MX
N 000314409                                                                     CEH
N 000314409
E 000314409 0001
E 12 009537 010771 010772 011281 012984 013029 017078 019263 021385 022827 022877 022878

----------------------------------------------------------------------------------------------------------------------------

N 000330541  3-(3,4-DICHLOROPHENYL)-1,1-DIMETHYL UREA (DIURON)                    6.0 MIL LBS  SRI  PESTICIDES
N 000330541
N 000330541 DIURON                                                                P
N 000330541                                                                     CEH
N 000330541 3-(3,4-DICHLOROPHENYL),-1,1-DIMETHYLUREA                           227
F 000330541 0001
E 0  005741 010961 013029 020762 021385 021526 022812 022827

----------------------------------------------------------------------------------------------------------------------------

N 000330552  3-(3,4-DICHLOROPHENYL)-1-METHOXY-1-METHYLUREA                        2.0 MIL LBS  SRI  PESTICIDES
N 000330552                                                                     CEH
N 000330552 MX8000655                                                            MX
N 000330552 LINURON                                                               P
N 000330552
E 000330552 0001
F 13 005094 008309 009537 010738 010771 010772 011281 013029 017078 020762 021385 022818 022827

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N 000333415  DIAZINON                                                            10.0 MIL LBS  SRI  PESTICIDES
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Table 3-1 (continued)

```
N 000333415
N 000333415ITHIOAT.                                                      11585  CEH
N 000333415 OO DIETHYL O-2-ISOPROPYL-4-METHYL -6-PYRIMIDINYL PHOSPHORIC 11585  CEH
N 000333415 DIAZINON                                                             P
E 000333415 0001
F 13 010178 012999 014190 016163 016302 016741 017984 020762 021385 021799 021918 022818 022827

------------------------------------------------------------------------------------------------------------

N 000510156  CHLOROBENZILATE                                           2.0 MIL LBS   SRI  PESTICIDES
N 000510156 CHLOROBENZILATE                                             FP
N 000510156
N 000510156                                                             CEH
N 000510156 4,4'-DICHLOROBENZILIC ACID, ETHYL ESTER                    212
N 000510156 CHLOROBENZILATE                                               P
F 000510156 0001
E 01 020762

------------------------------------------------------------------------------------------------------------

N 000532321  BENZOIC ACID, SODIUM SALT                                 13.3 MIL LBS   T72  MISC CHEMS
N 000532321                                                              MX
N 000532321 MX8000951                                                   CEH
N 000532321                                                              MX
N 000532321 MX8048984                                                    DC
N 000532321 SODIUM BENZOATE                                              FC
N 000532321 SODIUM BENZOATE                                              FC
N 000532321 SODIUM BENZOATE                                              MX
N 000532321 MX8046966                                                   KEM
N 000532321 SODIUM BENZOATE                                              NP
N 000532321 SODIUM BENZOATE                                              CO
N 000532321 SODIUM BENZOATE                                              CT
N 000532321 SODIUM BENZOATE                                              MX
N 000532321 MX8053529                                                    MX
N 000532321 MX8058433                                                    MX
N 000532321 MX8057316                                                    FA
N 000532321 SODIUM BENZOATE                                              MX
N 000532321 MX8047378                                                    MX
N 000532321 MX8025556
E 000532321 0001
E 01 010561

------------------------------------------------------------------------------------------------------------

N 000548265  PIGMENT RED 90                                            1.9 MIL LBS   T72  ORG PIGMENTS
N 000548265 D&C RED 22                                                 CI
N 000548265
N 000548265 BROMO ACID                                                 DC
N 000548265 MX8006948                                                  MX
F 000548265 0001
E 03 011621 013529 021904

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Table 3-3 (continued)

```
N 000563122  ETHION                                                             3.0 MIL LBS  SRI  PESTICIDES
N 000563122
N 000563122                                                                    CEH
N 000563122 ETHION                                                               P
E 000563122 0001
F 02 021385 022827

----------------------------------------------------------------------------------------------------------------------------------

N 000577117  SULFOSUCCINIC ACID, BIS(2-ETHYLHEXYL) ESTER, SODIUM SALT          12.4 MIL LBS  SRI  SURF-ACTIV AGENT     12.8 MIL LB
N 000577117 SULFOSUCCINIC ACID, BIS 2-ETHYLHEXYL ESTER, SODIUM SALT    15006  CEH
N 000577117 SODIUM DIOCTYL SULFOSUCCINATE                                       CT
N 000577117 DIOCTYL SODIUM SULFOSUCCINATE                                       CT
N 000577117 MX8050633                                                           MX
N 000577117 MX8049023                                                           MX
N 000577117 MX2012603                                                           MX
N 000577117 MX8059221                                                           MX
N 000577117 SODIUM DI-2-ETHYLHEXYL SULFOSUCCINATE                              KEM
N 000577117 MX8059641                                                           MX
N 000577117 MX8059630                                                           MX
N 000577117 MX8053494                                                           MX
N 000577117 SODIUM DIOCTYL SULFOSUCCINATE                                       FA
E 000577117 0001
E 02 006126 008026

----------------------------------------------------------------------------------------------------------------------------------

N 000657841  TOLUENESULFONIC ACID, SODIUM SALT                                  5.0 MIL LBS  SRI  SURF-ACTIV AGENT
N 000657841
F 000657841 0001
E 01 012672

----------------------------------------------------------------------------------------------------------------------------------

N 000709988  PROPANIL                                                           6.0 MIL LBS  SRI  PESTICIDES
N 000709988
N 000709988 PROPANIL                                                            FP
N 000709988 PROPANIL (ROGUE: STAM)                                               P
N 000709988                                                                    CEH
F 000709988 0001
E 06 005510 005695 013029 019529 021385 022827

----------------------------------------------------------------------------------------------------------------------------------

N 000759944  ETHYL N,N-DIPROPYLTHIOLCARBAMATE (EPTC)                            5.0 MIL LBS  SRI  PESTICIDES
N 000759944                                                                    CEH
N 000759944 MX8011607                                                           MX
N 000759944
N 000759944 EPTC (EPTAM)                                                         P
N 000759944 EPTC (EPTAM)                                                         P
F 000759944 0001
E 01 013029
```

Table 3-3 (continued)

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N 000915673  FD&C RED NO 2                                                     1.0 MIL LBS  T71  DYES
N 000915673
N 000915673 FD&C RED NO. 2  (AMARANTH)                                          C
N 000915673 AMARANTH SOLUTION                                                  CT
N 000915673 AMARANTH                                                            C
N 000915673 AMARANTH LAKE                                                       C
N 000915673 FD&C RED 2 (16185)                                                 CI
N 000915673 MX8052220                                                          MX
N 000915673 FD&C RED NO. 2                                                     FA
N 000915673 FD&C RED NO. 2 (AMARANTH)                                          FC
E 000915673 0001
F 09 013529 014892 017271 018778 019910 020784 020877 021285 022824

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N 000957517  N,N-DIMETHYL-2,2-DIPHENYLACETAMIDE                                3.0 MIL LBS  SRI  PESTICIDE
N 000957517
N 000957517 DIPHENAMIC                                                          P
N 000957517 DIPHENAMIC                                                          P
N 000957517                                                                   CEH
E 000957517 0001
F 05 012433 013029 021385 021799 022827

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Table 3-4

REFERENCES FOR CHEMICALS LISTED IN TABLE 3-3

SOURCE REFERENCE ACRONYM	REFERENCE
(blank)	Chemical Abstracts Service, American Chemical Society, The Common Data Base.
AR	Adhesives Red Book, Directory of the Adhesives Industry, published by Palmerton Publishing Company, Inc., New York, NY, pp. 161-219, 1972, 5th edition.
C	(1) J. Stephan Jellinek (translated from the German by G.L. Fenton), Formulation and Function of Cosmetics, Wiley Interscience, A Division of John Wiley and Sons, Inc., Princeton, NJ, Part 2, pp. 206-536, 1970. (2) Maison G. DeNevarre, The Chemistry and Manufacture of Cosmetics, D. Van Nostrand Company, Inc., Princeton, NJ, Vol. I, Background, pp. 181-238, 1962.
CD	R.A. Gosselin and Co., National Prescription Audit, General Information Report, Table 27, pp. 55-58.
CEH (some preceded by numbers)	Chemical Information Services, Stanford Research Institute, 1971 Directory of Chemical Producers, United States of America, Products Section, pp. 405-1009, 1971.
CI	Cosmetic, Toiletry and Fragrance Association, Inc., Certified Cosmetic Colors, revised March 10, 1972.
CT	Marion N. Gleason, Robert E. Gosselin, Harold C. Hodge, Roger P. Smith, Clinical Toxicology of Commercial Products, The Williams and Wilkins Co., Baltimore, MD, pp. 22-132, 1969.
DC	Drug and Cosmetic Catalog, 1973, published by Drug and Cosmetic Industry, New York, NY, Raw Material Directory, pp. 57-182, 1972.
FA	Thomas E. Furia, Editor, Handbook of Food Additives, published by the Chemical Rubber Co., Cleveland, OH, pp. 567-751, 1968.
FC	Food Protection Committee, Food and Nutrition Board, National Academy of Sciences / National Research Council, Chemicals Used in Food Processing, Publication 1274, National Academy of Sciences / National Research Council, Washington, D.C., 1965.
FDA	Code of Federal Regulations, Title 21, Office of the Federal Register, National Archives and Record Service, General Services Administration, Section 121.2502, p. 282; Section 121.2607, pp. 285-289; Section 121.2520, pp. 308-319; Section 121.2521, p. 320; Section 121.2526, pp. 326-333; Section 121.2535, pp. 344-345; Section 121.2550, pp. 357-359; Section 121.2553, p. 361; Section 121.2554; p. 362; Section 121.2575, p. 384; Section 121.2577, p. 385; Section 121.2578, p. 386, January 1, 1971, Revised.

Table 3-4 (continued)

FR	"Cancer Hazards Ranking and Information System Appendices," prepared for the National Cancer Institute, Bethesda, MD, Stanford Research Institute, Menlo Park, CA, Table E-2, pp. E-15-17; pp. E-23-24; Table E-4, pp. E-26-28; Table G-3, pp. G-13-14; Table F-5, p. F-10; Table F-1, p. F-6; Table F-2, p. F-7; Table F-4, p. F-9; Table H-4, pp, H-24-25; Table I-18B, pp. I-42-43; Table I-19, pp. I-45-61; Table J-2, pp. J-9-13; Table J-3, p. J-18 (Program Report November 1970 - October 1971).
HA	R.A. Gosselin and Co., National Prescription Audit, General Information Report, Table 32, pp. 70-71.
KEM	SRI Internal, Chemicals Used in Paint Formulations.
MX	Desktop Analysis Tool for the Common Data Base, American Chemical Society, PB 179-900, Vol. 5 of 6, Distributed by the Clearinghouse for Federal Scientific and Technical Information, Part A, Mixture/Component Cross-Reference Index, Mixtures Cross-Referred to Components, pp. A-1-43, 1968.
NF	Thomas E. Furia and Nicolo Bellanca (edited, translated, and revised), Fenaroli's Handbook of Flavor Ingredients, The Chemical Rubber Co., Cleveland, OH, Natural Flavors Section, pp. 33-256, 1971.
NP	Handbook of Non-Prescription Drugs, American Pharmaceutical Association, Washington, D.C., only tables listing component chemicals, 1971 edition.
P	Pesticides Monitoring Journal, Vol. 2, No. 1, Appendix, pp. 68-69, June 1968; Vol. 4, No. 3, Supplement III, pp. 163-166, December 1970; Vol. 5, No. 2, Appendix, p. 233, September 1971; Vol. 5, No. 4, Appendix, pp. 360-361, March 1972.
PA	R.A. Gosselin and Co., National Prescription Audit, General Information Report, Table 26, pp. 52-55.
PD	National Drug Code Directory, prepared by the Office of Scientific Coordination, Bureau of Drugs, Food and Drug Administration for Public Health Service, U.S. Department of HEW, Washington, D.C., Section B, pp. 1-22, June 1971.
PR	Paint Red Book, Directory of the Paint and Coatings Industry, published by Palmerton Publishing Company, Inc., New York, NY, pp. 239-340, 1971, 4th edition.
SF	Thomas E. Furia and Nicolo Bellanca (edited, translated, and revised), Fenaroli's Handbook of Flavor Ingredients, The Chemical Rubber Co., Cleveland, OH, Synthetic Flavors Section, pp. 259-640, 1971.

Table 3-4 (continued)

SLB	SRI Internal, New Chemicals Used in Food.
SO (preceded by a set of numbers and a single letter)	*SOCMA Handbook, Commercial Organic Chemical Names,* Chemical Abstracts Service, American Chemical Society, Part III, Text of Pure Chemicals, pp. 1-666, 1965.

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[*] In addition to chemicals selected for inclusion based on commercial significance and/or potential for human exposure, the Master Name Tape includes a group of chemicals which had been tested for carcinogenicity. The codes for these references follow:

(series of numbers)	Hartwell and Shubik, "Compounds Tested for Carcinogenic Activity"
HS	"

C. Evaluation of Mutagenicity Data on NSF Chemicals

With the aid of the list of 181 industrial chemicals referenced in the EMIC data base, the EPA Project Officer selected 25 chemicals for which SRI was to evaluate the mutagenicity on the basis of test results contained in the literature cited in the EMIC data base. These 25 chemicals are listed in Table 3-5. To carry out this analysis, SRI developed a list of assays considered to be relevant to prediction of the mutagenic potential of a chemical in mammals and a set of criteria for evaluating the test data from these assays. The list of assays and criteria were reviewed by the EPA Project Officer. The list of assays is given in Table 3-6 and the criteria are listed in Table 3-7.

The assays listed were chosen as being relevant to prediction of the potential of a chemical to cause genetic damage in mammals. In constructing the list, emphasis was placed on mammalian systems, both *in vivo* and *in vitro*, and on microbial systems involving the activation of the test chemical by mammalian metabolic enzymes. Assays in *Drosophila* and in microbial systems without metabolic activation were chosen on the basis of their widespread use in testing chemicals (e.g., the *Rec* Assay and the *E. Coli* WP2try$^-$ system). Assays in plants were not considered because of the difficulties inherent in interpreting the effects observed in terms of animal systems, and assays in phage were not considered because they have not been adequately characterized as measures of genetic damage. Because the literature to date covers essentially only tests of known carcinogens in these systems, assays of malignant transformation of cells in culture were also not included, but these assays may be a relevant future addition to the list.

The data evaluated came from literature on the selected chemicals which was cited in the EMIC data base. Each relevant article was indexed by an SRI Life Sciences professional who is familiar with the various mutagenicity test systems. Included in the indexing were such factors as the species and strain tested, the doses administered and dosage schedules, the route of administration or exposure to the chemical, the activity monitored and the activity level, data on positive and untreated controls, other information pertinent to the interpretation of the significance of the test (e.g., mammalian metabolic system used to activate a chemical tested in bacteria), and the author's interpretation of the results. The indexing was recorded on forms such as that of Figure 3-1, which covers cell system assays involving metabolic activation of the test chemical. Using the criteria listed in Table 3-7, the indexer evaluated each test as positive, negative, or inadequate. These evaluations and the relevant data were then reviewed by members of the Life Sciences staff with expertise in various areas of mutagenicity testing.

The results of all of the tests reviewed on each chemical were compiled and the chemical was classified as either (1) positive on the basis of having demonstrated mutagenic activity in at least one of the tests reviewed, or (2) negative/inadequate. Most of the chemicals in the second classification were placed there because they were judged to have been inadequately tested on the basis of the data presented in the reports reviewed. In many cases, the data presented were insufficient for evaluation. For example, dose-related activity was often not demonstrated, inactivity was reported at only a single dose, or it was not clear from the data reported that the test system was sensitive to the chemical (e.g., tests of water-insoluble chemicals in microbial assays requiring diffusion of the chemical through a water-based agar medium). It is possible that some of the tests classified as inadequate would have been classified as positive had the experimental data been reported in greater detail.

One important factor was not covered in the review--the possibility that the mutagenic activity observed could be caused by contaminants of the chemical under test which were engendered during synthesis, formulation, or storage. For example, commercial trichloroethylene is known to contain amine compounds as stabilizers, and it is possible that such stabilizers contribute to the weak mutagenic activity of the compound observed in *Escherichia coli* K-12 and *Salmonella typhimurium* in the presence of mammlian metabolizing systems. Unfortunately, in most of the tests reviewed, the purity of the chemical assayed could not be determined readily. That is, neither the manufacturer, the method of synthesis, nor the analytically-evaluated purity of the chemical was specified. In those cases in which the source of the chemical was identified, it was usually a chemical supply house, and no additional data on grade or purity were presented. For the few instances in which pertinent data on purity were presented, this information was included in the summary of the test.

The summaries on pages 3-89 through 3-180 are sequenced by chemical in ascending Chemical Abstracts Services (CAS) Registry Number order. For each chemical, brief tabulations of all of the positive and negative/inadequate tests reviewed and of the tests not reviewed are presented. The tests are described in more detail and the evaluations are explained in the text following this tabulation. For each test reviewed, the literature in which the data were reported is cited by EMIC accession number order. The full literature references in EMIC accession number order are found in a bibliography reproduced on pages 3-181 to 3-204.

Included among the tests not reviewed are those in plant systems, in phage, and those in which the genetic events monitored are not well characterized. Results of these tests were recorded in the summaries with references to the literature in which they were cited. The results were taken directly from the original articles or abstracts of the articles in which they were reported without evaluation. Review articles covering only previously published and reviewed data are referenced in the summaries without further evaluation.

Not all of the literature cited in the EMIC data base is directly related to mutagenicity testing. For example, in vitro reactions of the chemicals with nucleosides are considered peripheral to the subject of mutagenicity. This literature is cited in the summary by EMIC accession number only.

Table 3-5

COMPOUNDS FOR MUTAGENICITY EVALUATION

Chemical	CAS No.	Page No.
CARBON TETRACHLORIDE	56-23-5	3-89
ANILINE	62-53-3	3-93
BENZENE	71-43-2	3-97
IODOMETHANE (METHYL IODIDE)	74-88-4	3-103
ETHYLAMINE	75-04-7	3-105
ETHYLENE OXIDE	75-21-8	3-107
PROPYLENE OXIDE	75-56-9	3-113
TRICHLOROETHYLENE	79-01-6	3-116
N-NITROSODIPHENYLAMINE	86-30-6	3-119
BENZOYL PEROXIDE	94-36-0	3-123
o-DICHLOROBENZENE	95-50-1	3-126
NITROBENZENE	98-95-3	3-129
STYRENE	100-42-5	3-131
HEXAMETHYLENE TETRAMINE	100-97-0	3-135
EPICHLOROHYDRIN	106-89-8	3-139
ETHYLENE DIBROMIDE	106-93-4	3-146
ACRYLONITRILE	107-13-1	3-160
ETHYLENE GLYCOL	107-21-1	3-152
PHENOL	108-95-2	3-154
HYDROQUINONE	123-31-9	3-157
DIOXANE	123-91-1	3-162
BUTYLATED HYDROXY TOLUENE	128-37-0	3-164
THIRAM	137-26-8	3-170
ZIRAM	137-30-4	3-174
2-AMINOETHANOL	141-43-5	3-179

Table 3-6

MUTAGENICITY ASSAYS

I. Mammalian Systems

- A. In Vivo Treatment with Test Compound
  - 1. Induction of Point Mutations
    - Specific Locus Test (W. L. Russell)*
    - Nine Locus Biochemical Test (Valcovic and Malling)*
    - Histocompatibility Mutagen Test (Kohn)*
    - Spot Test (L. B. Russell)*
  - 2. Chromosome Damage or Rearrangement in Germ Cells
    - Dominant Lethal Assay (rat, mouse, males)
    - Heritable Translocation Test (males, mouse)*
    - Cytogenetic Analysis (general)
    - Unscheduled DNA Synthesis*
    - Sister Chromatid Exchange*
  - 3. Chromosome Damage or Rearrangement in Somatic Cells
    - Cytogenetic Analysis (general)
      - Bone Marrow
      - Peripheral Leukocytes
      - Fibroblasts*
      - Other
    - Unscheduled DNA Synthesis*
    - Micronucleus Test
    - Induction of Sex Chromosome Anomalies (L. B. Russell)*
- B. In Vitro Treatment with Test Compound (+/- Mammalian Metabolic Activation)
  - 1. Induction of Point Mutations
    - L5178Y(TK^+/TK^-)*
    - CHO Cells - Changes in Enzyme Electrophoretic Pattern (Siciliano and Humphrey)*
    - CHO Cells,* e.g.,
      - HGPRT Mutations
      - Ouabain Resistance Mutations
    - Chinese Hamster V-79 Cells, e.g.,
      - HGPRT Mutations (e.g., 8-Azaguanine Resistance)
    - Mouse L Cells*
      - Ouabain Resistance
    - Human Diploid Fibroblasts (WI-38),* e.g.,
      - HGPRT Mutations
      - APRT Mutations
  - 2. Chromosome Damage or Rearrangement
    - Sister Chromatid Exchange*
    - Unscheduled DNA Synthesis
    - Cytogenetic Analysis (general)
    - Alkaline Elution Assay

Table 3-6 (continued)

II. Host-Mediated Assays (test compound administered in vivo to mammalian host; mutagenic activity measured in non-mammalian or mammalian cell indicator after being metabolized by mammalian host)

A. Indicator Organism or Cell System Administered Intraperitoneally

Host: e.g., Mouse, Hamster,* Rat*

Indicators: e.g., Salmonella typhimurium (Ames' strains),
Neurospora crassa,*
Escherichia coli K-12*
Saccharomyces Cerevisiae D$_3$, D$_4$, D$_5$*
L5178Y Cells*
Schizosaccharomyces pombe P1
Serratia Marcescens

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes (e.g., urine, blood)*

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations (+/- Mammalian Metabolic Activation System)

Ames' Salmonella typhimurium histidine auxotrophs (reversion to his$^+$ in strains G-46, TA1535, TA1537, TA1538, TA98, TA100, etc.)
Escherichia coli tryptophan auxotrophs (reversion to try$^+$ in strains WP-2, WP2uvrA, WP67, CM611)
Neurospora crassa (forward mutations in heterkaryons at AD-3 loci)
Escherichia coli K-12 (galR^s/arg$^-$/NAD$^-$; both reversions and forward mutations tested)
Bacillus subtilis 168 Sporulation Mutants (MacGregor)*
Aspergillus nidulans (meth$_3^-$) - (reversion to methionine prototrophy)
Neurospora crassa strains W40 "distinctus" and 38701 (reversion to adenine prototrophy)
Escherichia coli strains Sd-B(TC), Sd-4-73, Sd-4 (reversions to streptomycin independence)
Escherichia coli (forward mutation to streptomycin resistance)*
Schizosaccharomyces pombe P1 (forward mutation to adenine dependence)
Klebsiella pneumonia (forward mutation to streptomycin resistance)
Serratia marcescens strains A21, A742, etc. (reversion to leucine prototrophy)
Saccharomyces cerevisiae 632/4 (reversion to methionine prototrophy)

Table 3-6 (continued)

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolic Activation System)

   PolA Disc Assay (Rosenkranz; comparison of inhibition of growth by test compound of *E. coli* W3110 (DNA polymerase A competent) and *E. coli* P3478 (DNA polymerase A deficient)

   Salmonella Repair Test (as above, comparison of inhibition of growth of repair deficient strain (e.g., *S. typhimurium* TA1535) and a similar, repair competent strain (e.g., *S. typhimurium* TA1975) by test compound)*

   Rec Assay (Kada; differential inhibition of growth of recombination deficient *Bacillus subtilis* M45 and recombination competent *B. subtilis* H17 in the presence of test compound). Other repair deficient strains of *B. subtilis* have been used in tests with repair competent *B. subtilis* 168.

   Saccharomyces cerevisiae
   - Mitotic Gene Conversion (strain D_4)
   - Mitotic Recombination (strains D_3 and D_5)

B. Drosophila

Induction of Sex-Linked Recessive Lethal Mutations

Introduction of Phenotypic Variants (e.g., Minutes and Bobbed Mutants)

Dominant Lethal Mutations (e.g., reduction in egg hatchability. A positive result in this test alone is not considered sufficient evidence of mutagenic activity).

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*Tests followed by an asterisk (*) were not found among the data reviewed for this study.

Table 3-7

CRITERIA FOR JUDGING THE ADEQUACY OF A MUTAGENICITY TEST

General Criteria for an Adequate Test

Activity monitored is a direct genetic effect or is a direct consequence of a genetic effect. The genetic event occurring is adequately characterized.

Activity appears to be a direct effect of the chemical or a metabolite of the chemical (e.g., there is evidence that the chemical reaches the genetic indicator and the test chemical is of sufficient purity that effects observed cannot be attributed to contaminants).

Activity observed is dose-dependent. This may be the single most important factor in determining if the effect observed is caused by the chemical.

For tests judged to be adequate and negative, the chemical is tested over a range of concentrations sufficient to detect any response.

Activity is reproducible (e.g., duplicate in vitro tests were run with small variations between results at same dose levels; standard deviation of response among animals tested at same dose level is low).

Activity is statistically significant compared to that of untreated controls and significant in itself in terms of the number of observations made. Untreated controls are run concomitantly.

Concomitant tests with known positive chemicals are run (with exception of systems involving human exposure to the chemical in vivo). This is most important in judging the adequacy of negative tests and in estimating the potency of weakly active chemicals (this criterion may be relaxed in judging tests having strongly positive results).

For assays in which the test compound is administered to a mammal in vivo, (1) there is evidence the chemical or its metabolites reach the indicator in the time allotted for the assay and (2) the route of administration is appropriate (e.g., in the standard host-mediated assay, the chemical and the indicator should not be administered by the same route).

Table 3-7 (continued)

General Criteria for an Adequate Test (continued)

For tests in which activity is measured in growing cells, cytotoxicity of the chemical and selection of mutant or wild type cells for growth is taken into account.

Criteria Specific to Certain Assay Systems and to Certain Chemicals

Examples of such criteria are listed below. These have been suggested by the SRI mutagenesis experts as they reviewed the data and were incorporated into the evaluations made in this study.

Dominant Lethal Assay

- Only males are treated with test chemical
- Induction of dominant lethals is demonstrated reproducibly and is dose-dependent during a single stage of spermatogenesis.
- Activity is considered to be a statistically significant incidence in dead implants over untreated controls, accompanied by a statistically significant reduction of live embryos.
- Extrapolation of effects observed after intraperitoneal administration of the test chemical to estimates of risks of human exposure is considered inappropriate.

Host-Mediated Assay

- Concomitant tests of the effect of the chemical on the indicator *in vitro* are run.
- The survival of the indicator in the host is taken into account in the calculation of activity.

Assays In Vitro with Mammalian Metabolizing Systems

- The activity of the mammalian metabolizing system is optimized.
- At least one of the positive controls tested requires metabolic activation to affect the genetic indicator.

Cytogenetic Analysis

- Gaps should not be included in tabulations of chromosome observations as they may be artifacts of preparing the chromosomes for analysis.
- The observations observed are classified by a standard nomenclature (e.g., Paris Conference, 1971, "Standardization in Human Cytogenetics," proceedings published by the March of Dimes National Foundation, New York, 1972).
- The number of samples per dose and the number of cells analyzed per sample are both adequate for statistical significance (e.g., 100 cells each from three samples may be better than 300 cells from a single sample).

Table 3-7 (continued)

Cytogenetic Analysis (continued)

- Mitotic arrest agents and stimulators are not used in excess concentrations or for excessively long periods of time.
- For tests *in vitro*, cells treated should not have been maintained for more than 50 passages.

Microbial Assays

- Exposure and expression times are such that spontaneous mutation frequencies are at their lowest and most nearly constant levels.

Figure 3-1

SAMPLE INDEXING FORMAT

IN VITRO
METABOLIC ACTIVATION

EMIC NO. ____________________

AUTHORS ____________________

____

REFERENCE____________________

I. COMPOUND

NAME ____________________

CAS NO.____________________

SYNTHESIS (e.g., MANUFACTURER) ____________________

IMPURITIES ____________________

METABOLITES IDENTIFIED ____________________

II. DOSE

AMOUNT/INCUBATION ____________________

VEHICLE ____________________

III. INDICATOR

SPECIES, STRAIN ____________________

CELL TYPE ____________________

NO. PER INCUBATION ____________________

GENETIC MARKER ____________________

MUTAGENIC RESPONSE ASSAYED ____________________

____

____

MECHANISM ____________________

____

IV. METABOLIC ACTIVATION SYSTEM

SPECIES, STRAIN ____________________

TISSUE ____________________

PRETREATMENT OF ANIMAL ____________________

____

Figure 3-1 (continued)

IV. METABOLIC ACTIVATION SYSTEM (Continued)

ADDITIONAL ENZYMES ________________

____

TYPE OF PREPARATION ________________

____

AMOUNT/INCUBATION ________________

____

V. TREATMENT

EXPOSURE TO TEST COMPOUND

PLATE ________ SPOT ________ LIQUID ________

METHOD OF INTRODUCING TEST COMPOUND ________________

____

LENGTH OF INCUBATION

WHOLE SYSTEM ________________

TEST COMPOUND & ACTIVATING SYSTEM (PRETREATMENT)

____

SPECIAL CONDITIONS ________________

GROWTH MEDIA ________________

SELECTIVE ________________

NON-SELECTIVE ________________

VI. RESULTS

A. SELECTIVE MEDIA ONLY OR ASSAY NOT INVOLVING GROWTH

(1) NO. OF MUTANTS (TREATED), M_t = ________________

(2) NO. OF MUTANTS (UNTREATED CONTROL), M_c = ________________

(3) $M_f = M_t - M_t$/CELLS PER PLATE = ________________

(4) M_f = OTHER METHOD) = ________________

B. BOTH SELECTIVE AND NON-SELECTIVE MEDIA

(1) NO. OF MUTANTS (TREATED-SELECTIVE MEDIA) = M_t = ________

(2) NO. OF MUTANTS (UNTREATED-SELECTIVE MEDIA) = M_c = ________

(3) NO. OF SURVIVORS (TREATED-NONSELECTIVE MEDIA) = S = ____

(4) $M_f = M_t - M_c/S$ = ________________

(5) M_f (OTHER METHOD) = ________________

Figure 3-1 (continued)

VI. RESULTS (Continued)

C. POSITIVE CONTROLS

COMPOUND ______________________

DOSE ______________________

M_f ______________________

COMPOUND ______________________

DOSE ______________________

M_f ______________________

D. M_f/nm TEST COMPOUND ______________________

VII. COMMENTS

AUTHOR'S INTERPRETATION

POSITIVE __________ NEGATIVE __________ ? __________

____

____

SRI INTERPRETATION

POSITIVE __________ NEGATIVE __________ ? __________

____

____

METABOLIC ACTIVATION ______________________

____

____

OTHER ______________________

____

____

Figure 3-1 (continued)

I. COMPOUND

METABOLITES IDENTIFIED--list by name only metabolites identified by the author as being formed via the metabolic activation system used in the assay described.

II. DOSE

AMOUNT/INCUBATION--if more than one dose is tested, write doses in ascending order, separated by commas with units immediately following the last dose (e.g., 0.5, 1.0, 5.0 ug/plate).

III. INDICATOR

SPECIES, STRAIN--format as follows (use abbreviations): S. TYPH TA100 or Mouse, DBA_2

CELL TYPE--for mammalian systems, identify by cell line (e.g., L5178Y) or by tissue of origin (e.g., kidney, epithelial)

NO. PER INCUBATION--don't calculate on first reading, if the value is not presented.

GENETIC MARKER--site on gene of activity being monitored (e.g., AD-3).

MUTAGENIC RESPONSE ASSAYED--e.g., reversion to histidine prototrophy

MECHANISM (if known)--e.g., forward mutation, reversion, base substitution and GC —— AT

IV. METABOLIC ACTIVATION SYSTEM

SPECIES, STRAIN--format as for Indicator

TISSUE--organ or tissue from which metabolic activation system is derived, e.g., liver.

PRETREATMENT OF ANIMAL--list any compounds and treatment used to induce metabolic enzymes, e.g., Arochlor 1254, IP, 500 mg/kg, 5 days before sacrifice.

ADDITIONAL ENZYMES--enzymes such as takadiase or sulfatase added to prepare the chemical for activation (e.g., to break down glucuronides) or enzymes added to supplement the activating system such as nitroreductase should be listed here.

TYPE OF PREPARATION--e.g., homogenate, purified microsomes or S-9 mix.

Figure 3-1 (continued)

V. TREATMENT

EXPOSURE TO TEST COMPOUND--check method by which indicator is exposed to test compound.

METHOD OF INTRODUCING TEST COMPOUND--for example, "as suspension directly onto plate or "embedded in filter paper disc."

INCUBATION TIME--Whole System is indicator, activating system, and test compound.

SPECIAL CONDITIONS--pH, temperature, aeration, out of light, etc.

GROWTH MEDIA (where applicable)--list names (e.g., Spizzizen's or Difco Nutrient Agar) if given; don't list separate ingredients unless necessary for interpretation of the assay results.

VI. RESULTS

Results should be listed in ascending order, corresponding to doses under II. If no value is given at a specific dose, put NA in appropriate space. Follow results with units where necessary (e.g., 100, 150, 200 revertants/plate).

M_f--Express as mutants/10^6 cells or survivors.

M_f (Other)--list algorithm used where known, use also for cases in which method of arriving at M_f is unknown.

POSITIVE CONTROL--list name of compound, doses, and results using formats described above.

On first reading, don't calculate values not listed in paper.

VII. COMMENTS

AUTHOR'S INTERPRETATION--Check POS/NEG/?; briefly describe author's judgment.

SRI INTERPRETATION--as above, use when author's interpretation is missing, equivocal, or when SRI disagrees. Typically, the SRI interpretation will disagree with that of the author in cases where the data presented is insufficient for establishing the results reported.

METABOLIC ACTIVATION--Yes, if activity is greater with metabolic activation than without. In explanation write a brief description of effect observed.

OTHER--to cover any pertinent information not listed above.

On first reading, do not calculate any parameters, just extract from author's tables. If a number comes from a graph rather than a table and is inexact, enclose it in parentheses.

June 1977

Classification:
Positive _____
Negative/Inadequate X

MUTAGENICITY EVALUATION
SUMMARY SHEET

COMPOUND: CARBON TETRACHLORIDE

CAS NO.: 56-23-5

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	Carbon tetrachloride was demonstrated to be inactive in inducing reversions to histidine prototrophy in Salmonella typhimurium strains TA100 and TA1535 with and without a mammalian metabolic activation system containing a rat liver microsome fraction. The chemical administered subcutaneously was reported to be inactive in a host-mediated assay in the mouse, with S. typhimurium strain G-46 as the indicator organism (incubated intraperitoneally in the mice), but no data were given on which to base an evaluation. Carbon tetrachloride was reported to be inactive in inducing reversions to histidine prototrophy in S. typhimurium strains G-46, TA1535, TA1538, and TA1950, and in inducing base-substitution mutations in Escherichia coli K-12 (gene loci monitored not specified) in the presence of a mammalian metabolic activation system containing a rat liver microsome fraction. No data were given on which to base evaluations of these tests.
Other Tests Not Reviewed:	Pretreatment of mice with carbon tetrachloride was reported to enhance the mutagenic activity of cyclophosphamide and to block the activity of diethylnitrosamine in inducing reversions to prototrophy in Salmonella typhimurium G-46 in the host-mediated assay in the mouse. Significant levels of polyploidy have been observed in regenerating liver cells of mice

treated with the chemical, but no increase in the incidence of chromosome aberrations has been seen.

Chromosome fragmentation was observed in root tips of Allium cepa treated with carbon tetrachloride.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-

2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally:

Carbon tetrachloride administered subcutaneously in a single dose of 4 ml/kg was reported to be inactive in inducing reversions to histidine prototrophy in *S. typhimurium* strain G-46 in the host-mediated assay in the mouse. However, no other data were given on which to base an evaluation (EMIC-20156).

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System:

Carbon tetrachloride at doses of 10-10^4 ug/plate, incorporated directly into agar medium plates containing the bacteria, was demonstrated to be inactive in inducing revertants to histidine prototrophy in *S. typhimurium* strains TA100 and TA1535 in the presence or absence of a mammalian metabolic activation system containing a microsome fraction (S-9) from the liver of rats pretreated with Aroclor 1254 to induce microsomal enzymes (EMIC-21337). Commenting on this test, the investigators suggested that this chemical may require a modified metabolic activation system for its detection as a mutagen (EMIC-21958).

Carbon tetrachloride was reported to be inactive in inducing reversions to histidine prototrophy in *S. typhimurium* G-46 and mutations (gene loci unspecified) in *Escherichia coli* K-12. The assays were carried out in the presence of a mammalian metabolic activation system containing liver microsomes from mice. The report is a meeting abstract and no data were presented on which to base an evaluation (EMIC-18910).

Carbon tetrachloride has been reported to be inactive in inducing base-substitution mutations in *E. coli* K-12 (no genetic marker was specified) and reversions to histidine prototrophy in *S. typhimurium* strains TA1535 and TA1538 in the presence of a mammalian metabolic activation system containing a rabbit liver microsome preparation. No data were reported on which to base evaluations of these tests (EMIC-21994).

The compound was also reported to be inactive in inducing reversions to histidine prototrophy in *S. typhimurium* strains G-46 and TA1950 in qualitative tests. No data on which to base evaluations of these assays were presented in the report (EMIC-20156).

b. No Mammalian Metabolizing System: -None-

2. Chromosome Damage or Rearrangement

   a. +/- Mammalian Metabolizing System: -None-

   b. No Mammalian Metabolizing System: -None-

B. *Drosophila*: -None-

IV. Results of Other Tests of Genetic Damage Reported in the Literature but Not Reviewed:

Pretreatment of mice with CCl_4 was reported to result in a significant increase in the mutagenic activity of cyclophosphamide in host-mediated assays using *S. typhimurium* G-46 as the indicator organism (EMIC-12961).

No increase in the level of chromosome aberrations was seen in the regenerating liver cells of mice treated with CCl_4 over that in mice induced to regenerate liver by partial hepatectomy (EMIC-4442). Significant levels of polyploidy have been observed in regenerating liver cells of mice intoxicated with CCl_4 (EMIC-8531, 8705, 8827, 14382, 23276).

Chromosome fragmentation was detected in Allium cepa root tips treated with CCl_4. Based on experiments in this study involving addition to and deletion of nucleic acids, the mode of action in inducing chromosome damage was hypothesized to be an effect on the metabolism of RNA (EMIC-10803).

In a study to develop standards for occupational exposure, cytogenetic effects of CCl_4 were evaluated. This study was cited in a meeting abstract, but no data were presented (EMIC-14069). The results of this study have not yet been published in the open literature.

Two review articles were published during 1976 in which the literature on the mutagenicity of CCl_4 is covered briefly (EMIC-23118, EMIC-23154).

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-4413, 4485, 12083, 13509, 15985, 16439, 17328, 20308, 20562, 21957, 22503)

June 1977

MUTAGENICITY EVALUATION
SUMMARY SHEET

Classification:
Positive ____
Negative/Inadequate _X_

COMPOUND: ANILINE

CAS NO.: 62-53-3

SUMMARY EVALUATION:

Positive Tests Reviewed:

None

Negative/Inadequate Tests Reviewed:

Aniline has been adequately demonstrated to be negative in *Salmonella typhimurium* strains TA1535, TA1537, TA100, and TA98 both in the presence and absence of a mammalian metabolic activation system containing a liver microsome fraction from rats pretreated with Aroclor 1254.

An increased incidence of chromosome aberrations was reported to be associated with aniline exposure in lymphocytes of four workers from a dyestuff factory. The sample size and data were inadequate for eliminating other causes of this effect.

The chemical was reported to be inactive in inducing chromosome damage as indicated by an alkaline elution assay of DNA from Chinese hamster lung fibroblasts (V-79) treated *in vitro*, but the qualitative data provided were insufficient for evaluation.

Aniline was also reported to be inactive in inducing reversions to prototrophy in *Aspergillus nidulans* (meth_3^-).

Freshly distilled aniline was reportedly approximately equally toxic to comparable DNA polymerase A deficient and competent strains of *Escherichia coli*, while commercial aniline and distillate allowed to stand for five days were more toxic to the polymerase deficient strain. Enhanced toxicity to the polymerase deficient strain may be indicative of potential for damaging DNA. Unfortunately, the data presented for this test and that for the test in Aspergillus were insufficient for evaluation.

Other Tests Not Reviewed:	Chromosome fragmentation has been observed in onion root tips treated with aniline.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Introduction of Point Mutations: -None-

2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells:

An increase in the percent of chromosome aberrations over that in unexposed controls was observed in lymphocytes from four workers in the dyestuff industry who had been exposed to aniline over periods of four to nine years. These results are presented because the increase in aberrations was significant for each of the workers, but evaluation is not feasible because the data reported and the sample size are inadequate for eliminating other possible causes (EMIC-17303).

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System):

No chromosome damage, as measured by the alkaline elution of fragmented DNA from polyvinyl filters, was observed in lysates of Chinese hamster lung fibroblasts which had been treated in culture with aniline at concentrations ranging from 0.03-3.0 mM. The cells were treated with aniline for 1,2, and 4 hours in the presence of an S-9 microsome fraction from rat liver (EMIC-23583). It is not yet feasible to assess fully the value of this technique in estimating the potential of a chemical to induce genetic damage as it has been used to study relatively few chemicals; however, it is included in the review since the positive results which have been obtained appear to correlate fairly well with assays of unscheduled DNA synthesis in other mammalian cell systems (Dr. A. D. Mitchell, SRI, personal communication). Unfortunately, it is not possible to adequately interpret the test of aniline, since only qualitative results were presented.

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System:

Aniline has been adequately demonstrated to be inactive in inducing revertants to histidine prototrophy in Salmonella typhimurium strains TA1535, TA1537, TA100, and TA98 (Ames' Salmonella/microsome Test). The chemical was tested over a wide range of concentrations in each strain (e.g., from 10 to 1000 μg per plate) and both in the presence and absence of a microsome fraction (S-9) from the livers of rats pretreated with Aroclor 1254 (EMIC-21337).

Aniline (at 200 μg/ml/4.26 x 10^6 conidia) has been reported to be inactive in reverting Aspergillus nidulans($meth_3^-$) to methionine independence. The data reported are insufficient for evaluating this test primarily because results at only a single dose were presented (EMIC - 5695).

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System:

A 25 μl dose of freshly distilled aniline was reported to be approximately equally toxic to DNA repair deficient Escherichia coli P3478 ($polA^-$) and repair competent E. coli W3110 ($polA^+$). In contrast, 25 μl of commercial aniline, tested in both the presence and absence of a rat liver homogenate, and 25 μl of aniline allowed to stand for five days after distillation were both more toxic to E. coli P3478 then to E. coli W3110. This greater toxicity to E. coli P3478 may be indicative of potential for inducing DNA damage. Unfortunately, the results reported are insufficient for evaluating the effect of aniline, primarily because data at only one dose level are presented. Also, it was suggested that the increased toxicity to strain P3478 in the presence of commercial product or distillate allowed to sit for five days was caused by oxidation products of aniline, but no data on the identity or activity of potential oxidation products were reported. Further, as noted by these investigators, the usefulness of this assay as a quantitative test may be questionable because of instability of the polA$^-$ mutant and difficulties in obtaining dose-response and in demonstrating reproducibility (EMIC- 24127).

b. No Mammalian Metabolizing System: -None-

B. Drosophila: -None-

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

The effects of aniline on mitosis in *Allium cepa* root tips were studied. At concentrations of 0.00005 to 0.01 M, constrictions appeared in chromosomes during late prophase or early metaphase. Occasionally, a section distal to the centromere broke off, producing a fragmented chromosome (EMIC-10652).

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-4630, 12660)

June 1977

Classification:
Positive _____
Negative/Inadequate _X[1]_

MUTAGENICITY EVALUATION
SUMMARY SHEET

COMPOUND: BENZENE

CAS NO.: 71-43-2

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	Benzene, administered intraperitoneally, was reported to be inactive in the dominant lethal assay in the rat, but no data were given on which to base an evaluation.

The chemical was reported to cause chromosome breaks and chromatid gaps in the bone marrow cells of rats and chromatid and isochromatid breaks and gaps in bone marrow cells of rabbits receiving subcutaneous injections of the chemical. Chromatid gaps were also observed in the leukocytes of rats, but gaps may not be a valid indicator of chromosomal damage. The data reported for these tests were insufficient for evaluation.

Benzene was also reported to cause a significant incidence of chromosome aberrations in peripheral blood and bone marrow cells, and a significant increase in micronuclei in polychromatic erythrocytes of rats given intraperitoneal injections of benzene. No data were given on which to base an evaluation.

In numerous case studies, chromosome aberrations (breaks, rings, and dicentrics) and aneuploidy have been reported to have been observed in blood cells of industrial workers exposed to benzene. Although the number of separate observations suggests a chromosome-damaging effect of benzene, the data presented in each study were insufficient for eliminating other possible causes of the aberrations.

---

[1] This classification of the published mutagenicity data on benzene is based on the inadequacy of the experimental methods in the individual tests reported. It should be noted that in a number of these tests, including studies on humans exposed to the chemical, benzene was reported to induce significant incidences of chromosome aberrations. Taken together, this body of data suggests that benzene may induce chromosome damage in animals and man.

The chemical was reported to cause chromatid, and chromosome breaks and gaps in cultured human leukocytes. Although the results were suggestive of a positive response, the data given were insufficient to establish the activity.

Benzene was reported to be inactive in inducing chromosome damage in cultured Chinese hamster lung fibroblast cells as measured by an alkaline elution assay of DNA, but no data were given on which to base an evaluation.

The compound, administered subcutaneously, was reported to be inactive in the host-mediated assay in the mouse using Salmonella typhimurium strain TA1950 as the indicator organism. No data were given on which to base an evaluation.

Benzene was also reported to be inactive in inducing reversions to histidine prototrophy in S. typhimurium strains TA100 and TA98 in the presence of a mammalian microscmal metabolic activation system, but no other data were given on which to base an evaluation.

Other Tests Not Reviewed: Benzene was reported not to cause aneuploidy or polyploidy in skin explants of mice painted with the chemical, but since the assays have not been established as indicators of potential for inducing chromosome damage, these tests were not reviewed.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. In vivo Treatment with Test Compound

1. Induction of Point Mutations: -None-

2. Chromosome Damage or Rearrangement in

a. Germ cells:

Benzene was reported to be inactive in the dominant lethal assay in male rats given the chemical intraperitoneally, but no data were given on which to base an evaluation (EMIC-23298[2]).

b. Somatic cells:

A high incidence of chromatid and isochromatid gaps and a low incidence of chromatid and isochromatid breaks were reported to have been observed in the bone marrow cells of rabbits which had received daily subcutaneous injections of benzene for an average of 18 weeks. However, since no control data were reported and no dose-response was demonstrated, and since gaps may not be a valid indicator of chromosome damage, the significance of this test is questionable (EMIC-12912).

A significant increase in the incidence of chromosome and chromatid deletions and gaps were seen in blood specimens, and double minutes and chromosome pycnosis were observed in bone marrow cells of rats which had received intraperitoneal injections of benzene. The chemical was also reported to cause a significant dose-related increase in micronuclei in polychromatic erythrocytes from bone marrow of treated rats. However, no data were given on which to base an evaluation (EMIC-23298[2]).

An increase in the incidence of chromosome breaks over that in untreated controls was observed within 24 hours of one or two subcutaneous injections of benzene (2.0, 4.0, or 6.0 ml/kg total dose). However, the significance of the results is not clear since there were only three animals per treatment group, only 50 cells monitored per animal, and a wide variation in aberration frequencies was noted among the animals in each group. Also, the absence of dose-response and criteria for scoring breaks discount the significance of the test (EMIC-7871).

Benzene was reported to cause chromosome breaks and chromatid gaps in bone marrow cells and chromatid gaps in leukocytes of rats. The cells were observed in metaphase 24 hours after the rats received a subcutaneous injection of the chemical (0.5, 1.0, or 2.0 ml/kg). No chromosome damage was observed 8 days after doses of 0.5 and 1.0 ml/kg in females. The data presented are insufficient for evaluation of the test as positive (at 24 hours after treatment), since dose-response was not demonstrated, gaps (which may be artifacts of the handling and staining of the cells) were used in tabulations establishing the significance of the aberrations, and data were reported for only one animal per treatment group (EMIC-6584).

The compound was reported to cause gaps and isochromatid and chromatid breaks in bone marrow cells of white neuter rats that had received twelve daily subcutaneous injections of the chemical. The incidence of aberrations reported was high (29% breaks, 26% gaps), but the test was considered inadequate since only eight animals were used, results at only one dose were reported, and no positive controls were included (EMIC-18215, see also EMIC-14737).

A number of case studies have been conducted on workers occupationally exposed to benzene. In the majority of the studies, cytogenetic analysis revealed a significantly higher incidence of chromosomal aberrations (mainly breaks, rings, and dicentrics) and aneuploidy among these workers than in unexposed controls (EMIC-5964, 6386, 6400, 7308, 7993, 8846, 11885, 14814, 18446, 18882). The significance of three studies was doubtful (EMIC-7729, 12722, 16030), and two could not be evaluated (EMIC-13307, 20447). No increase in aberrations was reported in one study (EMIC-15424). The studies cannot individually be used to document chromosome damaging effects of benzene, since workers may also have been exposed to other chemicals and other factors may have played a role (e.g., age or disease). However, when considered together, the evidence from these studies does suggest a potential chromosome-damaging effect of benzene in humans.

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System):

Benzene (ranging in concentration from 2.2×10^{-5} to 2.2×10^{-3} M) was reported to cause breaks and gaps in cultured human leukocytes; the incidence of aberrations ranged from 9.3 to 21.8%. However, only one sample was treated at each dose, dose-response was not adequately demonstrated, and no positive controls were included against which to compare the results. Also, breaks and gaps were scored together, without a separate listing of incidence of breaks alone. The test suggests a positive response, but since gaps may not be a valid measure of chromosome damage, the results reported are inconclusive (EMIC-19405).

Benzene at a concentration of 3×10^{-3} M caused a significant incidence of chromatid breaks in cultured human lymphocytes. When breaks and gaps were considered together, dose-response over a concentration range of 4.0×10^{-5} to 3.0×10^{-3} M could be demonstrated, but the gaps, a possible technical artifact, may not be a valid criterion of chromosome damage. No concomitant positive controls were run. Although the incidence of chromatid breaks at 3×10^{-3} M suggests a positive response, this single significant result is insufficient for interpreting the test as positive (EMIC-21381; see also EMIC-10254 for a limited study in human lymphocytes).

The chemical at a concentration of 10 mM was reported to cause no chromosome damage in Chinese hamster lung fibroblast (V79) cells as measured by an alkaline elution of fragmented DNA from treated cells. No data were reported on which to base an evaluation of this test. In addition, the assay has tested a relatively small number of chemicals so that its value in detecting chemically-induced DNA damage is not substantiated (EMIC-23583).

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally:

Benzene administered subcutaneously was reported to be inactive in a host-mediated assay in the mouse, with *S. typhimurium* strain TA1950 as the indicator organism, but no data were given on which to base an evaluation (EMIC-23298[2]).

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System:

Benzene was reported to be inactive in inducing reversions to histidine prototrophy in *S. typhimurium* strains TA100 and TA98 in the presence of a mammalian microsomal metabolic activation system, but no data were given on which to base an evaluation (EMIC-23298[2]).

b. No Mammalian Metabolizing System: -None-

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[2] The document cited is a dissertation abstract. On the basis of the material presented in the abstract, the reviewers judged procurement of the full dissertation to be unwarranted.

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System: -None-

B. Drosophila: -None-

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Aneuploidy was not detected in explants from the skin of newborn Swiss mice painted with benzene (EMIC-4762) and no doubled quadrupled, or octupled chromosomes were seen in skin explants of new Buffalo mice painted with benzene (EMIC-4846). These tests were not evaluated as the relationship of the effects assayed to the induction of chromosome damage has not been established. Also, these experiments were done before the analytic techniques presently used in cytogenetic studies had been developed.

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-4629, 4630, 4800, 4845, 4847, 4850, 4859, 7092, 9526, 11273, 12940, 12970, 15408, 20657, 21380, 22271, 22691).

June 1977

Classification:

Positive X

Negative/Inadequate ____

MUTAGENICITY EVALUATION

SUMMARY SHEET

COMPOUND: METHYL IODIDE

CAS NO.: 74-88-4

SUMMARY EVALUATION:

Positive Tests Reviewed:	Methyl iodide has been shown to be weakly active in inducing reversions to histidine prototrophy in *Salmonella typhimurium* TA100.
Negative/Inadequate Tests Reviewed:	Methyl iodide has been demonstrated to be inactive in inducing reversions to methionine independence in *Aspergillus nidulans* ($meth_3^-$).
Other Tests Not Reviewed:	None

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-
2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-
2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System:

Methyl iodide has been shown to be weakly active in inducing reversions to histidine prototrophy in _S. typhimurium_ TA100 when introduced as a gas into a desiccator holding open agar plates containing the bacteria. A dose-response relationship in this mutagenic activity has been observed (_EMIC_-21337; Dr. V. Simmon, SRI, unpublished results).

When added to a suspension of conidia and incubated for 5-40 minutes, methyl iodide in concentrations of 0.01-0.1 M has been demonstrated to be inactive in inducing reversions to methionine independence in _A. nidulans_ ($meth_3^-$) (_EMIC_-14842).

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System: -None-

B. _Drosophila_: -None-

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Evaluated: -None-

V. Peripheral Literature Cited in the EMIC Data Base:

Methyl iodide has been reported to induce local sarcomas in rats following subcutaneous administration (_EMIC_-7887; 8065).

Other peripheral literature: (_EMIC_-20273).

June 1977

MUTAGENICITY EVALUATION

SUMMARY SHEET

Classification:

Positive X (only with $NaNO_2$)

Negative/Inadequate ____

COMPOUND: ETHYLAMINE

CAS NO.: 75-04-7

SUMMARY EVALUATION:

Positive Tests Reviewed:	Ethylamine incubated with sodium nitrite was demonstrated to induce reversions to streptomycin independence in *Escherichia coli* Sd-4.
Negative/Inadequate Tests Reviewed:	In another study, ethylamine was observed to be inactive in inducing mutants in *E. coli* Sd-4, but no data were presented on which to base an evaluation of the test.
Other Tests Not Reviewed:	Ethylamine was reported to induce mitotic aberrations in sprouts of treated tomato seeds.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-

2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

   a. ± Mammalian Metabolizing System: -None-

   b. No Mammalian Metabolizing System:

A dose-related increase in the number of revertants to streptomycin independence was observed in *Escherichia coli* Sd-4 incubated for one hour with ethylamine (0.25, 0.5, and 1.0 M) and sodium nitrite at pH 6.4. The mutation frequency was significantly higher than either that observed for nitrite alone or for ethylamine alone. For example, ≈ 25 mutants/10^8 survivors were observed at 1.0 M ethylamine, ≈ 150 mutants/10^8 survivors at 0.5 M $NaNO_2$, and ≈ 1000 mutants/10^8 survivors at 1.0 M ethylamine plus 0.5 M $NaNO_2$. It was suggested that the potentiation of activity was a result of nitrosation of ethylamine to ethylnitrosamine, which is presumably converted to a reactive carbonium ion. A similar metabolic nitrosation of ingested amines and conversion to carbonium ions may occur in mammals (EMIC-17886).

In another study, ethylamine was reported to be inactive in inducing revertants to streptomycin independence in *E. coli* Sd-4, but no data were presented on which to evaluate the test (EMIC-5412).

2. Chromosome Damage or Rearrangement

   a. ± Mammalian Metabolizing System: -None-

   b. No Mammalian Metabolizing System: -None-

B. *Drosophila*: -None-

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Ethylamine at a concentration of 0.1% for 24 hours was reported to induce mitotic aberrations in sprouts of treated tomato seeds (EMIC-17493).

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-19343).

June 1977
rev. July 1977

MUTAGENICITY EVALUATION

SUMMARY SHEET

Classification:
Positive X
Negative/Inadequate ____

COMPOUND: ETHYLENE OXIDE

CAS NO.: 75-21-8

SUMMARY EVALUATION:

Positive Tests Reviewed:	Ethylene oxide has been demonstrated to induce reversions to histidine prototrophy in *Salmonella typhimurium* TA1535. The chemical was administered as a solution in cold ethanol to a suspension of the bacteria in phosphate buffer. A non-linear, dose-related increase in mutations was observed. The chemical was found to induce reversions to adenine prototrophy in *Neurospora crassa* W. 40 "distinctus" when administered directly into a conidial suspension as a gas dissolved in water. A limited dose-response was observed in the induction of mutations. Ethylene oxide has also been found to be weakly active in the induction of sex-linked recessive lethal mutations (Muller-5 Test) in *Drosophila melanogaster*. This activity has been confirmed in several studies and, in addition, the chemical has been found to induce minute mutants in *D. melanogaster*.
Negative/Inadequate Tests Reviewed:	Ethylene oxide was reported to induce dominant lethal mutations in rats and mice exposed by inhalation, but the data presented are insufficient for evaluation of these tests. The chemical has also been reported to induce chromosome aberrations in bone marrow cells from rats and mice exposed by inhalation. The data reported are inadequate for establishing these activities. The chemical was found to be inactive in the induction of hyperploidy (viable X fragments) in treated *D. melanogaster*. The evaluation of

this test was based on results reported for a single, high dose which had been optimized for detection of the chromosome aberrations and on the large number of chromosomes tested.

Other Tests Not Reviewed: Ethylene oxide has been reported to be inactive in the induction of reversions to methionine and glutamate prototrophy in *Streptomyces griseoflavus*, weakly active in inducing prophage in *Escherichia coli*, and inactive in inducing host-range mutations in bacteriophage T2h$^+$ and the parent bacteriophage T2. These tests were not reviewed because the mutational events occurring have not been adequately characterized as screens for genetic damage.

Mutants and chromosome aberrations have been detected in barley treated with ethylene oxide. Mutations have also been observed in vulgare wheat, *Eucalyptus*, and rice treated with the chemical, and chromosome aberrations have been observed in treated *Pterotheca falconeri*, *Tradescantia paludosa*, *Vicia faba*, and maize.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-

2. Chromosome Damage or Rearrangement in

a. Germ Cells:

Ethylene oxide, administered by inhalation at a single dose level of 1000 ppm for four hours, was reported to induce dominant lethal mutations in germ cells of male Long-Evans rats. Treated males were mated for 10 weeks to virgin females. Significant increases in dead implants/total implants over untreated controls were observed in pregnant females from weeks 1,2,3, and 5 of mating. This report is a meeting abstract and the data given are insufficient for evaluation. For example, no evidence of dose-response is presented and the parameters monitored are not tabulated (EMIC-20815).

Ethylene oxide, administered by inhalation at doses of 3.6 or 1112 mg/m^3 for 66 days, was reported to be active in the induction of dominant lethal mutations in male Albino mice. The data presented are insufficient for evaluation of this test. For example, dose-response at a single stage of spermatogenesis was not demonstrated. Also, experimental procedures such as the mating schedule were not documented (EMIC-23577; see also EMIC-16040, 18448).

b. Somatic Cells

Ethylene oxide was reported to be active in the induction of chromosome aberrations in bone marrow cells from mice exposed by inhalation to 3.6 or 112 mg/m^3 for 66 days. The data presented are insufficient for evaluation of the test, since the types of aberrations detected were not specified and experimental procedures (such as the number of animals treated and the number of cells analyzed) were not specified (EMIC-23577; see also EMIC-16040, 18448).

Significant increases in isochromatid gaps, chromatid gaps and breaks, rearrangements and exchanges, and ring formations were reported to have been observed in bone marrow cells from Long-Evans rats exposed by inhalation to 250 ppm ethylene oxide for 7 hrs/day for 3 days. The increase in total aberrations was from 7/120 metaphases analyzed in untreated controls to 101/120 metaphases analyzed in ethylene oxide-treated cells. Unfortunately, the report is a meeting abstract and the data presented are insufficient for evaluation of this test. For example, no dose-response data are presented, and the parameters monitored were not tabulated. Also, gaps, which may not reflect genetic damage, apparently were included in the total aberrations reported (EMIC-20815).

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System:

Administered as a solution in ethanol (0°C) directly into phosphate buffer (pH 7.4) containing the bacteria, ethylene oxide has been demonstrated to induce reversions to histidine prototrophy in S. typhimurium strain TA1535. A dose-response relationship (non-linear) was observed in mutation frequencies obtained on treatment of 2.9×10^8 bacteria with 0.96-95.5 mM ethylene oxide for 1 hr at 25°C. The mutation frequencies ranged from 2.47 ± 0.51 mutants/10^8 survivors at the lowest dose to 41.16 ± 3.30 mutants/10^8 survivors at the highest dose, compared to 2.36 ± 0.55 mutants/10^8 survivors in untreated controls (EMIC-21877; see also EMIC-21878).

Ethylene oxide has been demonstrated to induce reversions to adenine prototrophy in Neurospora crassa W. 40 "distinctus" when administered directly into the conidial suspension as a gas dissolved in water. A limited dose-response was reported. The mutation frequencies on treatment of 60×10^6 conidia were 27.0/10^6 survivors at 0.025 M ethylene oxide for 15 minutes and 144.0/10^6 survivors at 0.05 M for 10 minutes. The mutation frequency for the untreated controls was 0.13/10^6 survivors (the time of incubation was not specified) (EMIC-10610; see also EMIC-5101, 5106).

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System: -None-

B. Drosophila:

Ethylene oxide was found to be weakly active in the induction of sex-linked recessive lethal mutations (Muller-5 Test) and translocations in D. melanogaster. The chemical was administered to males by injection in single doses of a 0.055 or 0.09 M saline solution (EMIC-4946; see also EMIC-4535). This result was confirmed in another study in which ethylene oxide was found to be active in inducing sex-linked recessive lethals in D. melanogaster (Muller-5 Test) on injection of single doses of a 0.5 or 0.8% saline solution (EMIC-5044; see also EMIC-10863).

The chemical was also found to be active in inducing minute mutants (small chromosome deletions resulting in reduction of length and thickness of bristles) in D. melanogaster, but inactive in induction of hyperploids (viable X fragments) on injection of single doses of 113.6 mM. Although results were reported for only a single dose, the dose was optimized for comparison with the effects of other alkylating agents. Also, in both tests, a large number of chromosomes were analyzed (e.g., 1478 for the hyperploidy test) (EMIC-7357).

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Ethylene oxide was reported to be inactive in the induction of reversions to methionine and glutamate prototrophy in the fungus S. griseoflavus strains 21 and 28. These tests were not reviewed because the mutational events occurring were not adequately characterized as screens for genetic damage (EMIC-10759).

The chemical was reported to be weakly active in incuding prophage λ in E. coli K-12 (EMIC-20580), inactive in inducing host-range mutations in bacteriophage T2h$^+$ (EMIC-11883), and also inactive in inducing mutations in the parent bacteriophage T2 (EMIC-5606). These tests were also not reviewed because the events monitored were not characterized adequately as screens for genetic damage.

Ethylene oxide has also been reported to be mutagenic in several plant systems. Chromosome breaks (EMIC-5145), breviaristatum mutants (EMIC-21843), eceriferum mutants (EMIC-4641, 5379, 6304, 21483), and chlorophyll mutants (EMIC-21843) were observed in sprouts of barley seeds treated with ethylene oxide (see also EMIC-4925, 5782, 5783, 6917, 10855, 11473, 11803, and 13279). Mutations were observed in vulgare wheat (Triticum aestivum var. vulgare) after treatment of the seeds with ethylene oxide (EMIC-4642). Chromosome abberrations were detected in germinating seedlings of Pterotheca falconera treated with the chemical (EMIC-21748), and recessive mutations were detected in Eucalyptus species tereticornis, citriodoro, and malculata two generations after treatment of seedlings (EMIC-13400). Chromosome aberrations (e.g., chromatid breaks) were found in pollen grains of Tradescantia paludosa (EMIC-10868) and in root tips of Vicia faba (EMIC-9488) exposed to ethylene oxide. Chlorophyll mutations were found in rice after treatment of the seeds with the chemical (EMIC-17582, 20122, 20471, and 21770; see also EMIC-6591, 9557, 15857, and 15869). Chromosome aberrations have also been detected in maize treated with ethylene oxide (EMIC-10790, 16515).

In a study to develop standards for occupational exposure, cytogenetic effects of ethylene oxide were evaluated. This study was cited in a meeting abstract, but no data were presented (EMIC-14069). The results of this study have not yet been published in the open literature.

In a review article published in 1976, the mutagenicity data on the ethylene oxide was covered briefly (EMIC-23154).

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-7049, 9410, 10579, 11041, 12682, 13098, 21901)

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[1] (rev. July 1977). This experiment is reported in detail in the following recent journal article:

> Embree, J.W., Lyon, J.P., and Hine, C.H.,
> The Mutagenic Potential of Ethylene Oxide Using the Dominant Lethal Assay in Rats,
> Toxicol. Appl. Pharmacol. 40, 261-67, 1977 (EMIC -24861)

The data presented are still not adequate for demonstrating a positive effect in the dominant lethal assay, as results at only a single dose level (1000 ppm for 4 hrs) were reported.

June 1977

MUTAGENICITY EVALUATION

SUMMARY SHEET

Classification:

Positive _____

Negative/Inadequate X__

COMPOUND: PROPYLENE OXIDE

CAS NO.: 75-56-9

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	Propylene oxide was reported to be active in inducing reversions to adenine prototrophy in Neurospora crassa W. 40 "distinctus" A. This is the result of a single test in which the chemical was assayed at a dose chosen for optimal survival and mutagenicity. Propylene oxide was reported to be active in inducing sex-linked recessive lethal mutations in Drosphila melanogaster (Muller-5 Test). In this assay, mature sperm were treated by a post-copulatory douche in the female. The data presented were insufficient for evaluation of this test.
Other Tests Not Reviewed:	The chemical was reported to be inactive in inducing host-range mutations in bacteriophage $T2h^+$.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. In vivo Treatment with Test Compound

1. Induction of Point Mutations: -None-
2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System:

Propylene oxide has been demonstrated to induce reversions to adenine prototrophy in *Neurospora crassa* W. 40 "distinctus" A (from strain 38701). At the optimal concentration and time (0.5 M in a suspension containing approximately 132 x 10^6 conidia for one hour), the mutation frequency observed was 80/10^6 surviving conidia. In untreated controls after one hour of incubation, the mutation frequency was 0/10^6 survivors. Although a dose-survival relationship was established for propylene oxide during the optimization of the test concentration, there were no data reported indicating that a dose-response effect in induction of mutants had been observed (EMIC-5000).

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System: -None-

B. *Drosophila*:

Propylene oxide was reported to be active in inducing sex-linked recessive lethal mutations (Muller-5 Test) in *D. melanogaster* Oregon-K. *Drosophila* sperm were treated by a post-copulatory douche with the chemical. The mutation rate was 1.2% (13 lethals from 12 males/1074 tested) versus 0.06% (1 lethal/1650 tests) in untreated controls. Although the result suggests a positive effect, this report is essentially an abstract, and the data presented are insufficient for evaluation of this test (e.g., no demonstration of dose-response and inadequate description of the experimental method) (EMIC-5063).

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Propylene oxide (330 mM) was reported to be inactive in inducing host-range mutations in bacteriophage T2h^+. Mutants were identified as phage able to infect T2h^+-resistant *Escherichia coli* B/2 (EMIC-11883).

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-4993, 8407, 9179, 10869, 12998, 13215, 19048, 21077).

June 1977

Classification:
Positive X
Negative/Inadequate _____

MUTAGENICITY EVALUATION

SUMMARY SHEET

COMPOUND: TRICHLOROETHYLENE

CAS NO.: 79-01-6

SUMMARY EVALUATION:

Positive Tests Reviewed:	Trichloroethylene was found to be weakly active in inducing reversions to histidine prototrophy in *Salmonella typhimurium* TA100 in the presence of a mammalian metabolic activation system containing a microsome fraction (S-9) from the livers of B6C3F$_1$ mice pretreated with Aroclor 1254. These are unpublished results cited in a meeting abstract covered by this review (Dr. V. F. Simmon, SRI).
Negative/Inadequate Tests Reviewed:	In contrast to the activity seen in the study cited above, trichloroethylene was reported to be inactive in inducing reversions to prototrophy in *S. typhimurium* TA100 in the presence of a mammalian metabolic activation system containing the S-9 microsome fraction from livers of mice (strain not specified) pretreated with phenobarbitone. The data presented are insufficient for evaluation of this test. The chemical was reported to be active in inducing reversions to arginine independence and weakly active in inducing mutations to ability to metabolize galactose in *Escherichia coli* K-12 (strain not specified, but presumably 343/113 or one of its derivatives). In the same strain, the chemical was reported to be inactive in inducing reversions to NAD$^+$ prototrophy and forward mutations to 5-methyltryptophan resistance. All of these tests were carried out in the presence of a mammalian metabolic activation system containing liver microsomes from mice pretreated with phenobarbital. The data presented are insufficient for establishing the results reported.
Other Tests Not Reviewed:	None

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-

2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System:

Trichloroethylene was found to be weakly active in inducing reversions to histidine prototrophy in *S. typhimurium* TA100 in the presence of a mammalian metabolic activation system containing a microsome fraction (S-9) from the livers of B6C3F$_1$ mice pretreated with Aroclor 1254. Agar plates containing the bacteria were exposed to a vapor of trichloroethylene for one hour at 37°C. A dose-related increase in revertants was observed over the concentration range 0.8-2.0% (Dr. V. F. Simmon, SRI, unpublished results; cited in *EMIC*-21978).

In contrast, trichloroethylene, also administered as a gaseous mixture in air to agar plates containing the bacteria, was reported to be inactive in inducing reversions to histidine prototrophy in *S. typhimurium* TA100. The tests were carried out in the presence of a microsome fraction (S-9) from the livers of mice pretreated with phenobarbitone, either with or without an NADPH generating system. Time and dose-dependency data were reported to have been obtained, but were not presented. Moreover, the report is a meeting abstract and the data presented are insufficient for evaluation of the test (EMIC-22111).

Trichloroethylene was tested in *E. coli* K-12 (strain not specified, but presumably 343/113 or a derivative thereof) for ability to induce mutations at the *galR*^{s} locus, to induce reversions to arginine and NAD$^+$ prototrophy, and to induce forward mutations to 5-methyltryptophan resistance. In the presence of a mammalian metabolic activation system containing liver microsomes from mice pretreated with phenobarbital, the chemical at a single, 3 mM concentration, was reported to be active in inducing reversions to arginine prototrophy, very slightly active in inducing mutations at *galR*^{s}, and inactive at the other two loci. The data presented are insufficient for evaluating either the positive or negative tests, primarily because results at only a single dose are reported, the mutagenic responses observed were of borderline significance (approximately 2.3 x the spontaneous rate at the *arg* operon and 1.23 x the spontaneous rate at *galR*^{S}), and none of the actual mutations for either treated or control bacteria were tabulated (EMIC-21339).

b. No Mammalian Metabolizing System: -None-

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System: -None-

B. *Drosophila*: -None-

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

In a review article published in 1976, mutagenicity data on trichloroethylene were covered briefly (EMIC-23118).

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-4630, 21321, 23149).

June 1977

MUTAGENICITY EVALUATION

SUMMARY SHEET

Classification:

Positive ____

Negative/Inadequate X

COMPOUND: N-NITROSODIPHENYLAMINE

CAS NO.: 86-30-6

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	N-Nitrosodiphenylamine has been demonstrated to be inactive in inducing reversions to histidine prototrophy in *Salmonella typhimurium* TA100, TA98, TA1535, and TA1537 in the presence or absence of a mammalian metabolic activation system containing a rat liver microsome fraction (S-9). Similarly, the chemical has been found to be inactive in inducing reversions to streptomycin independence in *Escherichia coli* B6 strain Sd-B(TC) in the presence of a mammalian metabolic activation system containing either purified microsomes or cell sap from rat liver. The chemical was also reported to be inactive in inducing reversions to histidine prototrophy in *S. typhimurium* TA1530 in the presence or absence of a rat liver microsome fraction and in inducing reversions to streptomycin independence in *E. coli* Sd-4-73. No data were presented on which to base an evaluation of these tests. The chemical was reported to be inactive in inducing reversions to adenine prototrophy in *Neurospora crassa* 38701, but the data presented were insufficient for evaluation.
Other Tests Not Reviewed:	Chromosome aberrations have been detected in the root tips of *Vicia faba* treated with N-nitrosodiphenylamine in the presence of light and acridine orange, but not in root tips treated with N-nitrosodiphenylamine alone.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

  A. In vivo Treatment with Test Compound

    1. Induction of Point Mutations: -None-

    2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

  B. In vitro Treatment with Test Compound

    1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

    2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

  A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

  B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

  A. Microbial Systems

    1. Induction of Point Mutations

      a. +/- Mammalian Metabolizing System:

Incorporated into the agar containing the bacteria, N-nitrosodiphenylamine at concentrations ranging from 10 to 500 μg/plate was demonstrated to be inactive in inducing reversions to histidine prototrophy in S. typhimurium strains TA100, TA98, TA1535, and TA1537 in the presence or absence of a mammalian metabolic activation system containing a microsome fraction (S-9) from the livers of rats pretreated with Aroclor 1254. The investigators reporting these data caution that testing of this compound was incomplete because of toxicity to the bacteria at higher doses (EMIC-21337; see also EMIC-23922). N-Nitrosodiphenylamine has also been found to be inactive in these strains of S. typhimurium when pre-incubation of the bacteria, chemical, and metabolic activation system was carried out in liquid suspension (Dr. V. Simmon, SRI, unpublished results). Recently, the compound was found to be inactive in S. typhimurium TA100 on pre-incubation in liquid suspension at concentrations up to and greater than 1 μmole/ approximately 10^8 bacteria. The incubations were carried out in the presence of a microsome fraction from livers of rats pretreated with pentobarbital (Yahagi, et al., 1977[1]).

N-Nitrosodiphenylamine has been demonstrated to be inactive in inducing reversions to streptomycin independence in E. coli B6 strain Sd-B(TC) in the presence of rat liver metabolic activation systems. No increase in the number of revertants per 10^8 survivors over that in untreated controls was observed in bacteria exposed to the chemical at 0.05 mM/10^9 cells (the highest dose compatible with at least 30% survival, which these investigators defined as the minimum level at which mutations could be detected with adequate statistical significance) in the presence of purified microsomes or a liver cell sap preparation (supernatant from centrifugation at 10,000 × g for 30 minutes). No data were reported from tests done without the mammalian metabolic activation systems (EMIC-17876).

This chemical was reported to be inactive in inducing reversions to histidine prototrophy in S. typhimurium TA1530 in the presence or absence of a metabolic activation system containing a microsome fraction from rat liver. The test was carried out both in a liquid pre-incubation system and directly in soft agar plates. No data were presented on which to base an evaluation (EMIC-23116).

b. No Mammalian Metabolizing System:

N-Nitrosodiphenylamine was reported to be inactive in inducing reversions to streptomycin independence in E. coli Sd-4-73. No data were presented on which to base an evaluation of this test (EMIC-5412).

At a 1 mM dose N-nitrosodiphenylamine was reported to be inactive in inducing reversions to adenine prototrophy in Neurospora crassa 38701 exposed for 30 minutes. The data reported are insufficient for evaluation, primarily because results at only a single dose were presented and no concomitant tests of positive controls were reported (EMIC-8333).

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System: -None-

B. Drosophila: -None-

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Chromosome aberrations have been detected in the root tips of *Vicia faba* treated with N-nitrosodiphenylamine in the presence of light and acridine orange (*EMIC*-8323). No aberrations were seen in root tips treated with N-nitrosodiphenylamine alone (*EMIC*-8324).

V. Peripheral Literature Cited in the EMIC Data Base:

N-Nitrosodiphenylamine was reported to be non-carcinogenic when administered to rats by stomach tube at a dose level equivalent to 400 μg dimethylnitrosamine daily, five days per week for 52 weeks (*EMIC*-8517).

Other peripheral literature: (*EMIC*-23169).

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[1] Yahagi, T., Nagao, M., Seino, Y., Matsushima, T., Sugimura, T., and Okada, M., *Mutat*. *Res*. *48*, 121-130, 1977.

June 1977

Classification:
Positive ____
Negative/Inadequate X

MUTAGENICITY EVALUATION
SUMMARY SHEET

COMPOUND: BENZOYL PEROXIDE

CAS NO.: 94-36-0

SUMMARY EVALUATION:

Positive Tests Reviewed: None

Negative/Inadequate Tests Reviewed:

Benzoyl peroxide was reported to be inactive in inducing dominant lethal mutations in the mouse, but the data reported were insufficient for adequate evaluation of the test. Also, the route of administration, which was intraperitoneal, may not be appropriate in estimating the effect of the chemical in humans.

Benzoyl peroxide was reported to be non-toxic to both repair deficient *Escherichia coli* P3478 (pol A^-) and repair competent *E. coli* W3110 (pol A^+). Greater toxicity to strain P3478 may be indicative of potential for inducing DNA damage. Unfortunately, the data reported are insufficient for establishing the negative result.

Other Tests Not Reviewed:

Benzoyl peroxide was reported to be inactive in inducing streptomycin and penicillin resistance in *Micrococcus pyogenes* var. *aureus* FDA 209, but the tests were not reviewed because the mutagenic events being monitored were not adequately characterized.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-

2. Chromosome Damage or Rearrangement in a) *Germ Cells* and b) Somatic Cells:

   Benzoyl peroxide, administered intraperitoneally (34 and 52 mg/kg) to male ICR/HA mice, was reported to be inactive in inducing dominant lethal mutations. This report is essentially a review article and the data presented are insufficient for evaluation of the results. For example, none of the implant or fetal death counts are presented. Although the chemical was tested at two doses, the significance of the difference between the two amounts is questionable. Also, the effect of the chemical after intraperitoneal injection may not be relevant to effects in humans after exposure. Inhalation and ingestion may have been more appropriate routes of administration (*EMIC*-12984).

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangemet n (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

   a. +/- Mammalian Metabolizing System: -None-

   b. No Mammalian Metabolizing System: -None-

2. Chromosome Damage or Rearrangement

   a. + Mammalian Metabolizing System: -None-

   b. No Mammalian Metabolizing System:

      A 500 μg dose of benzoyl peroxide was reported to be nontoxic to both *E. coli* P3478 (pol A^-) and *E. coli* W3110 (pol A^+). Greater toxicity to strain P3478 may be indicative of potential for inducing DNA damage. The results reported are insufficient for establishing inactivity, primarily because data at only one dose level are presented. That toxicity was not detected in either strain may be a result of the inability of benzoyl peroxide to penetrate the agar to reach the bacteria (EMIC-24127).

B. Drosophilia: -None-

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Benzoyl peroxide was reported to be inactive in inducing streptomycin and penicillin resistance in *Micrococcus pyogenes* var. *aureus* FDA 209. These tests were not reviewed because the mutations monitored were not characterized adequately (EMIC-11162).

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-4616).

June 1977

Classification:

Positive ____

Negative/Inadequate X

MUTAGENICITY EVALUATION
SUMMARY SHEET

COMPOUND: o-DICHLOROBENZENE

CAS NO.: 95-50-1

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	o-Dichlorobenzene was reported to be inactive in inducing reversions to histidine prototrophy in *Salmonella typhimurium* (8 strains, not identified). The data reported were insufficient for evaluation of the tests. Also, the assays were spot tests, and the method used may be inappropriate for detecting activity with o-dichlorobenzene. The chemical was reported to induce a very slight increase in the frequency of reversion to methionine prototrophy in *Aspergillus nidulans* ($meth_3^-$). The data reported are insufficient for evaluating the significance of this result.
Other Tests Not Reviewed:	None

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-
2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System:

o-Dichlorobenzene, applied directly to the surface of solidified agar media containing the bacteria, was reported to be inactive in inducing reversions to prototrophy in 8 histidine-requiring strains of *S. typhimurium* (strains were not specified) at single doses of 1-5 µl. No other data were given on which to base an evaluation of this test, and since *o*-dichlorobenzene is insoluble in water, it is not clear that it was able to diffuse through the agar to reach the bacteria, as is required for an adequate test by this procedure (*EMIC*-13029).

When incubated with a suspension of the spores in saline at a dose of 200 µg/ml for 60 minutes, *o*-dichlorobenzene was reported to increase the frequency of reversion to methionine prototrophy in *A. nidulans* ($meth_3^-$) from $3/10^6$ spores (untreated controls) to $5/10^6$ spores. No results at other doses or other data are reported on which to base an evaluation of the significance of this result, except that *meta*- and *para*-dichlorobenzene induced higher mutation frequencies ($9/10^6$ spores and $11/10^6$ spores, respectively) and 3,4-dichloroaniline induced a mutation frequency of $60/10^6$ spores in this test at the same dose and exposure time (*EMIC*-5170, 5695).

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System: -None-

B. *Drosophila*: None

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed: -None-

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-4629)

June 1977

Classification:

Positive _____

Negative/Inadequate X

MUTAGENICITY EVALUATION
SUMMARY SHEET

COMPOUND: NITROBENZENE

CAS NO.: 98-95-3

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	Nitrobenzene has been reported to induce a low but significant level of recessive lethal mutations in *Drosophila melanogaster* when administered as a vapor. The data presented are insufficient for evaluation of the test.
Other Tests Not Evaluated:	None

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-
2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-
2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues or Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System: -None-

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System: -None-

B. Drosophila:

Nitrobenzene was reported to induce sex-linked recessive lethal mutations in *Drosophila melanogaster* when administered as a vapor for 8-10 days. The incidence was 4% of chromosomes analyzed compared to 0.14% of chromosomes from untreated controls. No other data were presented on which to base an evaluation of the test (EMIC-10783).

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed: -None-

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-4630, 18236).

June 1977

MUTAGENICITY EVALUATION

SUMMARY SHEET

Classification:

Positive _____

Negative/Inadequate __X__

COMPOUND: STYRENE

CAS NO.: 100-42-5

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	Styrene was reported to be inactive in inducing forward mutations to 8-azaguanine resistance in Chinese hamster cells (V79), in inducing reversions to histidine prototrophy in qualitative tests in *Salmonella typhimurium* strains TA1535, TA1537, TA1538, TA98, and TA100, and in inducing sex-linked recessive lethal mutations in *Drosophila melanogaster*. The data reported for these tests were insufficient for establishing inactivity.

Styrene was also reported to be inactive in inducing forward mutations to adenine dependence in *Schizosaccharomyces pombe* P_1 either in the presence or absence of a mammalian metabolic activation system containing purified mouse liver microsomes, but it was not clear from the data presented that a sufficient quantity of activated metabolites was produced in the incubation system. The question of efficiency of the activation system is raised because there have been other studies indicating that styrene may be metabolized to a mutagen.

For example, sytrene was reported to be active in host-mediated assays in the mouse using *Schizosaccharomyces pombe* P_1 (forward mutation to adenine dependence) and *Saccharomyces cerevisiae* D_4 (mitotic gene conversion at the *ade*$_2$ and *trp*$_5$ loci) as indicator organisms. The chemical was administered by gavage and the yeast were incubated intraperitoneally in these tests. Unfortunately, the data presented were insufficient for establishing activity.

Also, styrene oxide, a major human metabolite of styrene, has been demonstrated to be active in inducing mutations to 8-azaguanine resistance in

Chinese hamster cells (V79), in inducing adenine-dependent mutants in Schizosaccharomyces pombe P_1, mitotic gene conversion in Saccharomyces cerevisiae D_4, and in inducing reversions to histidine prototrophy in S. typhimurium TA100. Styrene oxide was also reported to be active in a qualitative test for the induction of reversions to histidine prototrophy in S. typhimurium TA1535 and in host-mediated assays in the mouse using the test systems described above for styrene, but the data reported for these tests were inadequate for establishing activity.

Other Tests Not Reviewed:	None

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. In vivo Treatment with Test Compound

1. Induction of Point Mutations: -None-
2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

B. In vitro Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System):

Styrene (8.5, 17.0 mM) was reported to be active in inducing forward mutations to 8-azaguanine resistance in Chinese hamster cells (V79) exposed for one hour at 37°C. The data presented were inadequate for establishing inactivity, primarily because results at only two doses were presented, and the doses tested covered only a twofold concentration range. In the same system, styrene oxide, a major human metabolite of styrene, was found to induce a dose-related increase in mutations when tested at concentrations of 4.25, 8.50, 17.0, and 25.0 mM (EMIC-21995, 23911).

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally:

Styrene was reported to be active in host-mediated assays in the mouse using Schizosaccharomyces pombe P_1 and Saccharomyces cerevisiae D_4 as the indicator organisms. The chemical was administered as a single 1000 mg/kg (1 ml of a solution in DMSO) dose by stomach tube, and the effects monitored were forward mutation to adenine dependence in *Saccharomyces pombe* P_1 and mitotic gene conversion at *ade*$_2$ and *trp*$_5$ in *Saccharomyces cerevisiae* D_4. The data presented were insufficient for establishing activity, primarily because dose-response was not demonstrated. Also, the maximum mutation frequency observed in *Schizosaccharomyces pombe* P_1 (after 12 hours of incubation) and the maximum conversion frequency observed at the *trp*$_5$ locus in *Saccharomyces cerevisiae* D_4 (after 6 hours incubation) were of borderline significance, being approximately twice those of untreated controls. The maximum conversion frequency observed at the *ade*$_2$ locus of the *Saccharomyces* (after 6 hours of incubation) was markedly positive, being four to fivefold higher than that in untreated controls. Styrene oxide (100 mg/kg) was reported to be active in the same test systems, but these data were also insufficient for establishing activity because of the single dose tested and because the maximal activities observed at all three loci were of borderline significance (*EMIC*-21955, 23911).

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System:

Styrene (100 mM/10^8 yeast/assay mix) was reported to be inactive in inducing forward mutations to adenine dependence in *Schizosaccharomyces pombe* P_1 either in the presence or absence of mammalian metabolic activation system containing purified microsomes from the livers of Swiss albino mice. The chemical, yeast, and activation system were incubated together for one hour in liquid suspension at 37°C. The data presented are inadequate for establishing inactivity, primarily because the tests were carried out at a single dose and treatment time, and no evidence was presented that these parameters had been optimized for detection of mutants.

In the same study, styrene oxide, at concentrations of 5.0, 10.0, 15.0, and 20.0 mM, was found to induce a dose-related increase in the number of adenine mutants over that in zero-time controls in *Schizosaccharomyces pombe* P_1 exposed for one hour at 37°C without metabolic activation (*EMIC*-21995, 23911).

b. No Mammalian Metabolizing System:

Styrene, applied as a 5 µl (approx. 500 µg) drop directly onto the hardened surface of agar plates containing the bacteria, was reported to be inactive in inducing revertants to histidine prototrophy in *Salmonella typhimurium* strains TA100 and TA1535. These were qualitative tests carried out at a single, high dose and, therefore, not adequate for establishing a negative result. Styrene oxide was also tested and was active in qualitative tests in both strain TA1535 and TA100. It was shown to induce a dose-related increase in revertants in strain TA100 when spotted on the hardened agar containing the bacteria or applied to the lids of petri dishes containing the bacteria in doses of 50, 200, and 500 µg. Higher activity was observed when the chemical was applied to the lid of the petri dish, indicating that it was better dispersed to the bacteria as a vapor than by diffusion through the agar. Both styrene and styrene oxide were tested by the qualitative spot method at single doses of 5 µl and reported to be inactive in inducing reversions to histidine prototrophy in *S. typhimurium* strains TA1537, TA1538, and TA98 (*EMIC*-21384).

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System:

Styrene oxide was found to be active in inducing gene convertants to adenine independence in *Saccharomyces cerevisiae* D_4. No tests with styrene in this system *in vitro* were reported (*EMIC*-23911).

B. *Drosophila*:

Styrene was reported to be inactive in the induction of sex-linked recessive lethal mutations in *Drosophila melanogaster* (ClB/W Test). This report was essentially an editorial review and no data were presented on which to base an evaluation of the test (*EMIC*-18783).

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed: -None-

V. Peripheral Literature Cited in the EMIC Data Base: -None-

June 1977

MUTAGENICITY EVALUATION

SUMMARY SHEET

Classification:

Positive ____

Negative/Inadequate X

COMPOUND: HEXAMETHYLENETETRAMINE

CAS NO.: 100-97-0

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	Hexamethylenetetramine was reported to induce dominant lethal mutations in mice when administered orally at a dose of 25,000 mg/kg-bw. The chemical was reported to be inactive in inducing dominant lethal mutations in mice when administered in single intraperitoneal doses of 800, 1000, 1200, or 1500 mg/kg, and in single, intraperitoneal doses of 10,000 and 25,000 mg/kg (the compound is highly toxic at this dose by this route of administration). The data presented are insufficient for establishing the results reported. The chemical was reported to induce chromosome aberrations in HeLa cells and human lymphocytes treated in culture. In both tests, the data reported were insufficient for establishing activity, primarily because effects were observed only at single, high doses. Hexamethylenetetramine was reported to be more toxic to DNA repair deficient *Escherichia coli* p3478 (Pol A^-) than to repair competent *E. coli* W3110 (Pol A^+). Greater toxicity to strain p3478 may be indicative of potential for inducing DNA damage. The data from this test are also insufficient for establishing a positive effect, as the enhanced toxicity was recorded at a single, high dose. The chemical was reported to be mutagenic in *Drosophila melanogaster*, but the data presented are insufficient for evaluation of this test.
Other Tests Not Reviewed:	Hexamethylenetetramine was reported to induce sterility mutants in *Aspergillus niger*.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-

2. Chromosome Damage or Rearrangement in a) *Germ Cells* and b) Somatic Cells:

Hexamethylenetetramine, on oral administration of a single dose of 25,000 mg/kg-bw, was reported to be active in inducing dominant lethal mutations in male C3H mice. Each treated male was mated to three virgin females weekly for 8 weeks, and the pregnant females were sacrificed and analyzed 13.5 - 15.5 days after observation of a vaginal plug. No stage of spermatogenesis was specifically sensitive to the chemical. In this study, hexamethylenetetramine was also tested in C3Hx101F_1 mice at 10 g/kg by intraperitoneal injection and in C3H mice at 25 g/kg by intraperitoneal injection (the chemical was highly toxic at this dose by this route of administration). The chemical was reported to be inactive in these tests. The data for all three tests are inadequate for establishing the effects reported, primarily because results at only single doses are presented. Also, adequate demonstration of a positive result would have required a dose-related increase in the incidence of dominant lethals at a specific stage of spermatogenesis (*EMIC*-5273, 7306, 11378).

The same investigators reported a preliminary study in which hexamethylenetetramine was inactive in inducing dominant lethal mutations in C3H mice given single, intraperitoneal injections of 800, 1000, 1200, and 1500 mg/kg. No other data were presented on which to base an evaluation, and the dose range tested (only a twofold increase overall) was inadequate for establishing inactivity. Also, intraperitoneal administration may not be a relevant route of exposure in estimating the potential effects of a chemical on humans. The oral route used in the formal study may have been more appropriate (*EMIC*-5273, 7306).

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System):

Hexamethylenetetramine was reported to induce chromosome aberrations (fragments, deletions, and breaks) in HeLa cells treated in culture at a concentration of 1×10^{-3}M for 16 hours. No aberrations were seen in tests at 1×10^{-5} or

1×10^{-4}M. The data were inadequate for establishing a positive result, primarily because a significant response was observed at only a single dose (EMIC-7306).

Hexamethylenetetramine at maximum tolerated doses was reported to induce chromosome aberrations in human lymphocytes treated in culture, but no aberrations were seen in cells treated with doses in the therapeutic range. This report is essentially a review article and no data are presented on which to base an evaluation of these tests (EMIC-5274).

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System:

A 6 mg dose of hexamethylenetetramine was reported to be more toxic to *E. coli* P3478 (Pol A^-) than to *E. coli* W3110 (Pol A^+). Greater toxicity to strain P3478 may be indicative of potential for inducing DNA damage. The results reported are insufficient for establishing activity, primarily because no data indicating a dose-response are presented (the compound was tested at two doses, 500 µg and 6 mg, but toxicity was observed only at the higher dose). It was suggested that the activity observed was in response to formaldehyde, a potential degradation product of hexamethylenetetramine, but no data on the activity of formaldehyde are reported to substantiate this hypothesis. It should also be noted, as suggested by these investigators, that the usefulness of this test as a quantitative assay may be questionable because of the instability of the $PolA^-$ mutant and difficulties in demonstrating reproducibility (EMIC-24127).

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-
b. No Mammalian Metabolizing System: -None-

B. *Drosophila*:

Hexamethylenetetramine (30-50 mg or 100 mg vapor) and its calcium chloride salt (0.5, 2.0 g vapor) were reported to be inactive in inducing mutations in *Drosophila melanogaster*, when insects were treated in either the larval or imago stages of metamorphosis. The data presented are inadequate for establishing a negative result because the dose levels tested for each chemical covered only a narrow range (three- to four-fold maximum differential), the number of chromosomes analyzed was small, and the experimental methods were not adequately detailed (i.e., the types of mutations monitored were not specified) (EMIC-4585).

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Hexamethylenetetramine was reported to induce sterility mutants in *Aspergillus niger*. The study was not reviewed, primarily because the mutational event monitored has not been adequately characterized (EMIC-8633).

V. Peripheral Literature Cited in the EMIC Data Base: -None-

June 1977

MUTAGENICITY EVALUATION
SUMMARY SHEET

Classification:
Positive X
Negative/Inadequate ____

COMPOUND: EPICHLOROHYDRIN

CAS NO.: 106-89-8

SUMMARY EVALUATION:

Positive Tests Reviewed:

Epichlorohydrin has been shown to induce chromosome aberrations in bone marrow of female ICR mice treated *in vivo* and in human lymphocytes treated *in vitro*.

The chemical has also been shown to be active in a host-mediated assay in ICR female mice using *Salmonella typhimurium* strains G-46, TA100, and TA1950 as indicator organisms. Induction of reversions to histidine prototrophy was the mutational event monitored in the *Salmonella*; the chemical was administered intramuscularly (using strains TA100 or G-46 as indicators) or subcutaneously (using TA1950 as the indicator); and the bacteria were incubated in the peritoneal cavity of the mice.

Epichlorohydrin has been demonstrated to induce reversions to histidine prototrophy in *S. typhimurium* strains G-46 and TA100, reversions to tryptophan prototrophy in *Escherichia coli* B/r (*try*$^-$), and reversions to adenine prototrophy in *Neurospora crassa* W.40 "distinctus" A in tests *in vitro*.

Negative/Inadequate Tests Reviewed:

Epichlorohydrin was reported to be inactive in a dominant lethal assay in male ICR/HA Swiss mice. The data presented are inadequate for evaluation of the test. Also the route of administration used (intraperitoneal) may not be relevant to estimating the risks of human exposure.

An increase in the percent of chromosome aberrations was reported to have been observed in lymphocytes from a group of workers after a year of exposure to epichlorohydrin. The data presented are preliminary and insufficient for evaluation of the effect of the chemical.

In host-mediated assays in female ICR/HA Swiss mice, the chemical was found to be inactive when S. typhimurium strains TA1951 and TA1952 were used as indicator organisms. As described above for the positive assays, the mutational event monitored in the Salmonella was reversion to histidine prototrophy; the chemical was administered subcutaneously; and the bacteria were incubated in the peritoneal cavity of the mice.

In qualitative tests in vitro, epichlorohydrin was reported to be inactive in inducing reversions to histidine prototrophy in S. typhimurium strains TA1534, TA1537, TA1538, TA1950, TA1951, and TA1952. The data presented and the methods used are inadequate for establishing the negative results, but inactivity in strains TA1534, TA1537, TA1538, TA1951, and TA1952 might be predicted, since these strains are designed to detect frameshift mutagens and epichlorohydrin would be expected to be more active in inducing base-substitution mutations.

Epichlorohydrin was reported to be non-toxic to both DNA repair competent Bacillus subtilis 168 and repair deficient B. subtilis strains MC-1, FB-13, and HCR-9. Greater toxicity to any of the repair deficient strains than to the repair competent strain may be indicative of potential for inducing DNA damage. The data presented are insufficient for evaluation.

In meeting abstracts, epichlorohydrin was reported to be mutagenic in unspecified strains of S. typhimurium and Escherichia coli and in inducing forward mutations to streptomycin resistance in Klebsiella pneumoniae. No data were presented on which to base evaluations.

Other Tests Not Reviewed:

Epichlorohydrin has been reported to induce mutations to nitrous acid sensitivity in Saccharomyces cerevisiae 55R5 and to be inactive in inducing streptomycin and phage resistance in Xanthomonas phaseoli var. fuscans. The chemical has also been reported to have been used in a variety of microorganisms (i.e., strains of Streptomyces, Penicillium, Arthrobacter, and Cephalosporium) to induce mutations which improve antibiotic production. The mutational events occurring in these studies are not adequately characterized for evaluation as measures of the gene-damaging potential of epichlorohydrin.

The chemical has been reported to induce chromosome aberrations in root tips of Vicia faba and at eceriferum loci in barley.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-

2. Chromosome Damage or Rearrangement in

a) Germ Cells:

Administered intraperitoneally in a single dose of 150 mg/kg, epichlorohydrin was reported to be inactive in inducing dominant lethal mutations in male ICR/HA Swiss mice. The data presented are insufficient for evaluation of this test, primarily because results at only a single dose were reported and none of the parameters used to detect dominant lethals were tabulated (e.g., early fetal deaths and total implants). Also, effects observed after intraperitoneal administration may not be relevant to effects observed in humans exposed to the chemical. Inhalation or ingestion may have been more appropriate routes of administration (*EMIC*-12984).

b) Somatic Cells:

Epichlorohydrin has been demonstrated to induce a dose-related increase in the incidence of chromosome aberrations over that observed in untreated controls in bone marrow cells from treated, female ICR/HA mice. Dose-response was observed at 24 hours after intraperitoneal administration of single doses between 1 and 20 mg/kg and oral administration of single doses of 5 and 20 mg/kg. Significant incidences of chromosome breaks were also observed 6, 24, and 48 hours after single intraperitoneal doses of 50 mg/kg; 6 hours after five intraperitoneal doses (in 7 days) of 5, 10, and 20 mg/kg; 6 hours after five doses (one per day) of 10 mg/kg; 24 hours after a single oral dose of 40 mg/kg; 6, 24, and 48 hours after a single oral dose of 100 mg/kg; 6 hours after five oral doses (in 7 days) of 20 mg/kg; and 6 days after five (one per day) oral doses of 20 mg/kg. The number of animals tested per dose and the statistical analysis of the data were not reported (*EMIC*-23532).

An increase in the percent of chromosome aberrations in lymphocytes was observed in workers exposed to epichlorohydrin for a year. These preliminary data are from a prospective study in which the control is the blood of the same workers before exposure. Unfortunately, the data presented were insufficient for evaluation of the effect of epichlorohydrin because the number of workers tested and the number of cells analyzed per worker were not specified, and the blood samples were pooled rather than tested separately for each worker (*EMIC*-24116).

B. In vitro Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System):

Epichlorohydrin has been demonstrated to induce a limited, dose-related increase in the percentage of chromosome aberrations (primarily chromatid breaks) over that in untreated controls in human lymphocytes (pooled from one male and one female) treated in culture with 10^{-8} - 10^{-5}M epichlorohydrin. These results were obtained in lymphocytes treated during the last 24 hours of cultivation. The cells were analyzed in metaphase (EMIC-21912, 23532).

These investigators also applied a banding technique to the analysis of cytogenetic effects of epichlorohydrin in human lymphocytes. Using essentially the banding method of Burkholder and Comings (Exptl. Cell Research 75, 268-71, 1972) which involves trypsinization of metaphase chromosome preparations followed by Giemsa staining, a significant increase in the percent of chromosome aberrations over that in solvent controls was observed in the lymphocytes treated in culture with 10^{-6}M epichlorohydrin for the last 24 hours of cultivation. The breaks observed showed non-random distribution among the chromosomes. For example, breaks in the 9q12 chromosome segment were observed significantly more frequently than in other segments, and the whole Y chomosome appeared to be insensitive to breaks. The percentage of aberrations was far higher than that observed by the conventional technique at the same concentration (28% by banding vs. 2.0% by conventional staining; in untreated controls, 4.0% aberrations were detected by banding vs. 1.0% by conventional staining). It should be noted that the higher number of breaks observed by banding could be an artifact of the technique (e.g., gaps may appear to be breaks) as well as a result of increased sensitivity in detecting aberrations. Ideally, the numbers of breaks detected would have been the same by both methods (EMIC-20626, 21913).

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally:

Epichlorohydrin has been demonstrated to be active in the host-mediated assay in female, ICR mice using *S. typhimurium* G-46, TA100, and TA1950 as indicator organisms. A limited dose-response relationship was demonstrated in the induction of reversions to histidine prototrophy in these strains. Following incubation for three hours after single intramuscular (for G-46 and TA100) or subcutaneous (TA1950) injections of 50 and 100 mg/kg of the chemical in DMSO[1], mutation frequencies greater than those in controls were observed in all three strains, with the values at 100 mg/kg higher than those at 50 mg/kg. The investigators reporting these data considered the mutation frequencies obtained at 100 mg/kg (which were 5.09, 3.50, and 2 x M_f in untreated controls for G-46, TA100, and TA1950 respectively) to be significantly positive. In similar assays at the same doses, no activity was detected in inducing reversions to histidine prototrophy in S. typhimurium strains TA1951 and TA1952. No positive controls were reported. Epichlorohydrin was also found to be mutagenic in vitro in strains G-46 and TA100 (EMIC-23532).

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[1] DMSO = dimethyl sulfoxide.

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System:

Epichlorohydrin has been demonstrated to induce reversions to histidine prototrophy in S. typhimurium strains G-46 and TA100. The bacteria were exposed to the chemical for 60 minutes and dose-related increases in mutations were observed over the concentration range of 1.08×10^{-3} - 1.08×10^{-1}M in strain G-46 and 1.08×10^{-3} - 5.4×10^{-2}M in strain TA100. The method of exposing the bacteria to the compound was not specified and the dose-response effect observed was not linear. In spot tests in which 50 µl of solutions of 1, 10, 50, and 100% epichlorohydrin (solvent not specified) were applied to hardened top agar containing the bacteria, reversions to histidine prototrophy were observed in S. typhimurium strain G-46 at 10, 50, and 100% and in strain TA100 at 1 and 10%. No reversions were seen in other strains tested at these concentrations (TA1950, TA1951, TA1952, TA1534, TA1537, TA1538). Since epichlorohydrin is insoluble in water, it is not certain that it diffuses through agar to reach the bacteria; hence, the reliability of this spot technique in testing the compound is questionable. The negative results in strains TA1534, TA1537, TA1538, TA1951, and TA1952 might have been predicted since these strains best detect frameshift mutations and epichlorohydrin would be expected to be more active in inducing base-substitution mutations (EMIC-23532).

In a second study, epichlorohydrin (in DMSO), incorporated into molten top agar containing the bacteria, was shown to be active in inducing reversions to histidine prototrophy in S. typhimurium TA100. The activity was demonstrated to be dose-related over the range 25.6 - 500 µM.

It should be noted that since epichlorohydrin is volatile, incorporation into molten agar may be a less effective technique for treating the bacteria than would be exposure to a vapor of the chemical (EMIC-23138).

The toxicities of epichlorohydrin to B. subtilis strains 168 (wild type), MC-1 (hcr^+, rec^-), FB-13 (uvr^-, rec^+), and HCR-9 (hcr^-, rec^+) were tested. Greater toxicity to any of the repair deficient strains than to the wild type may be indicative of potential to induce DNA damage. In these tests, epichlorohydrin (as a 0.113M solution in DMSO) was applied to filter paper discs which were then placed directly on agar plates containing the bacteria. No growth inhibition was observed in any strain. The data presented are insufficient for evaluation, since results at only a single dose were reported and the lack of inhibition in any strain raises the possibility that the chemical was unable to diffuse through the agar to reach the bacteria (EMIC-23138).

Epichlorohydrin has been shown to induce reversions to tryptophan prototrophy in E. coli B/r (try^-). The compound was tested as 0.6 ml of a 1:1 ethanol solution which was added to a suspension of 7×10^8 bacteria in 50 ml 0.1M phosphate buffer (pH 7.2). Although results at only a single dose were presented, the test is judged to be positive since significant activity was observed in several trials involving treatment times ranging from 0 to 25 minutes and expression on several media (e.g., minimal media, minimal media plus glutamic acid, minimal media plus glutamic acid and 0.05% broth). Also the mutational event monitored has been well characterized (see Schwartz, N. and Strauss, B., Nature 182, 888, 1958 and Demerec, M. and Cahn, E., J. Bacteriol. 65, 27-36, 1953) (EMIC-6982).

Another group of investigators reported epichlorohydrin to be mutagenic in S. typhimurium and E. coli (strains not specified) (EMIC-16208). Also, the chemical was reported to induce forward mutations to streptomycin resistance in Klebsiella pneumoniae (EMIC-13640). Both of these reports are meeting abstracts, and no data are presented on which to base evaluations.

Epichlorohydrin has been demonstrated to induce reversions to adenine prototrophy in Neurospora crassa W.40 "distinctus" A. Although dose-response data were not reported, the results presented were obtained at an optimal dose (a concentration yielding approximately 50% survival after 45 minutes exposure) and incubation time (the treatment time yielding the highest percentage of mutants). For epichlorohydrin a mutation frequency of 135.2 revertants/10^6 survivors was observed on one hour of treatment of 73.6×10^6 conidia at a concentration of 0.15M chemical in water (EMIC-5000).

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Epichlorohydrin has been reported to induce mutations to nitrous acid sensitivity in *Saccharomyces cerevisiae* 55R5 (EMIC-21777) and to be inactive in inducing streptomycin resistance and phage resistance in *Xanthomonas phaseoli* var. *fuscans* (EMIC-11454). These tests were not evaluated as the systems were inadequately characterized as screens for the induction of genetic damage.

The chemical is reported to have been used to induce mutations which improve antibiotic production in a number of microorganisms, namely *Penicillium chrysogenum*, *Streptomyces nodosus*, *Streptomyces noursei*, *Streptomyces umbrinus*, *Streptomyces prasinus*, *Streptomyces roseochromogenes*, and *Arthrobacter simplex* (EMIC-9212), and *Cephalosporium acremonium* (EMIC-22526). These mutations are also inadequately characterized for evaluation of these tests as screens for the gene-damaging potential of epichlorohydrin.

Epichlorohydrin has been reported to induce chromosome aberrations in root tip meristems of *Vicia faba* (EMIC-9488) and mutations at *eceriferum* loci in barley (EMIC-4641).

In a monograph published in 1976, mutagenicity data on epichlorohydrin were reviewed briefly (EMIC-23118).

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-9179).

June 1977

Classification:
Positive X
Negative/Inadequate ____

MUTAGENICITY EVALUATION

SUMMARY SHEET

COMPOUND: ETHYLENE DIBROMIDE (EDB)

CAS NO.: 106-93-4

SUMMARY EVALUATION:

Positive Tests Reviewed:	Ethylene dibromide was shown to induce unscheduled DNA repair in cultured opossum lymphocytes. The chemical was shown to be active in the host-mediated assay in the mouse using *Salmonella typhimurium* G-46 as the indicator organism. Induction of reversions to histidine prototrophy was the mutational event monitored in the *Salmonella*; the chemical was administered intramuscularly; and the bacteria were incubated in the peritoneal cavity of the mouse. (In a qualitative test, ethylene dibromide was also reported to be active in inducing mutations in *S. typhimurium* G-46 *in vitro*.) The compound was demonstrated to be weakly active in inducing reversions to histidine prototrophy in *S. typhimurium* strains TA1530, TA1535, and TA100, to induce forward mutations at the Ad-3 gene locus (to a requirement for adenine) in *Neurospora crassa*, and to be highly active in inducing mitotic gene conversion in *Saccharomyces cerevisiae* D_4. Ethylene dibromide was also shown to be active in inducing sex-linked recessive lethal mutations in *Drosophila melanogaster*. These mutations were observed specifically in spermatids and spermatocytes.
Negative/Inadequate Tests Reviewed:	The chemical was reported to be inactive in inducing chromosome breakage in human lymphocytes. No data were given on which to base an evaluation of this test. Ethylene dibromide was found to be inactive in inducing deletions in the *gal-chl* gene region of *S. typhimurium* LT-2. The compound was reported to be inactive in the dominant lethal test in the mouse following intraperitoneal or oral administration. The data presented were insufficient for an adequate evaluation of this test.

Ethylene dibromide was reported to be inactive in inducing reversions to leucine prototrophy in *Serratia marcescens* A21 in the host-mediated assay in the mouse. The chemical was administered intramuscularly and the bacteria, intraperitoneally. However, the data given were insufficient for establishing a negative result. The compound was also reported to be inactive *in vitro* in a qualitative test with *S. marcescens*, but no data were given on which to base an evaluation.

The chemical was reported to be inactive in inducing reversions to histidine prototrophy in *S. typhimurium* strain TA1538. The data presented and the methods used were inadequate for establishing the negative result, the inactivity in strain TA1538 would be predicted since this strain is designed to detect frameshift mutations and ethylene dibromide would be expected to be more active in inducing base-substitution mutations.

Ethylene dibromide was reported to be more toxic to repair deficient *Escherichia coli* P3478 (pol A$^-$) than to repair competent *E. coli* W3110 (pol A$^+$). Greater toxicity to strain P3478 may indicate potential for inducing DNA damage. The data reported were insufficient for evaluating the effect of ethylene dibromide.

Other Tests Not Reviewed:

Ethylene dibromide was reported to cause pink somatic mutations in stamen hair cells of *Tradescantia* mutable clones *02*, *0106*, and *4430*.

The compound was reported to be mutagenic in barley kernels, but not to cause chromosome breaks in root tips of *Allium*.

Evaluation of Tests Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-

2. Chromosome Damage or Rearrangement in a) *Germ Cells* and b) Somatic Cells:

Ethylene dibromide was reported to be inactive in inducing mutations when administered intraperitoneally (18 or 90 mg/kg) or orally (5 times, 50 or 100 mg/kg) to male ICR/HA Swiss mice. This report is essentially a review article and the data presented were insufficient for establishing a negative result, primarily because none of the relevant parameters were tabulated (e.g. total implants, early fetal deaths, and pregnancy rates) (EMIC-12984).

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System):

Ethylene dibromide (10^{-6} - 10^{-2}M/15 x 10^6 cells) was found to induce unscheduled DNA synthesis (UDS) in opossum lymphocytes treated for one hour. Although positive and negative control values were not given, the results are considered positive since the effect observed was dose-related and the level of UDS was greater than that induced by either methyl- or ethylmethanesulfonate (EMIC-17827).

The compound was reported to be inactive in inducing chromosome breakage in human lymphocytes. This report was a meeting abstract and no data were presented on which to base an evaluation (EMIC-20037).

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally:

Ethylene dibromide has been reported to cause reversions to histidine prototrophy in *S. typhimurium* G-46 in the host-mediated assay in mice. In this test a single high dose of 500 mg/kg was administered intramuscularly to the mice and the bacteria were incubated in the peritoneal cavity. The mutation frequency was $6.23/10^8$ vs. $0.77/10^8$ in untreated controls. Because of the high mutation frequency relative to that of controls, the test is judged to be positive with the reservation that the activity was reported only for a single high dose in only 6 animals, and there were no data presented to indicate dose-response. As it was also reported to be active *in vitro* (in a qualitative test) there is no evidence that mammalian metabolism affected the mutagenicity of ethylene dibromide in *S. typhimurium* G-46 (EMIC-13608, 14101).

In contrast, the chemical administered intramuscularly was reported to be inactive in inducing reversions to leucine prototrophy in *Serratia marcescens* A21 in the host-mediated assay in the mouse. The compound was also reported to be inactive in *S. marcescens* in a qualitative test *in vitro*. The data presented are insufficient for evaluating the effect of ethylene dibromide in the host-mediated assay with *S. marcescens*, since results at only a single dose were reported for only 6 animals (EMIC-13608, 14101).

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. ± Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System:

Administered as a liquid directly into molten agar containing the bacteria, ethylene dibromide has been shown to be weakly active in inducing reversions to histidine prototrophy in S. typhimurium TA1535 and TA100. The activity was linearly dose-related, and the test was carried out without a mammalian metabolic activation system (EMIC-21337). Since ethylene dibromide is volatile, application into molten agar may not be the optimal mode of exposure. Higher mutation frequencies are observed in the Salmonella when ethylene dibromide is placed on a filter disc and then laid on the agar, or when the plates containing the bacteria are exposed to the compound as a vapor (Dr. V. F. Simmon, SRI, personal communication).

In qualitative tests, ethylene dibromide has been shown to be active in inducing reversions to histidine prototrophy in S. typhimurium strains TA1530 and TA1535. In these tests, 10 µl of the chemical were applied to a filter paper disc, which was then laid on hardened agar containing the bacteria. Using the same technique for exposing the bacteria to ethylene dibromide, a linear, dose-related increase in mutagenic activity over a range of approximately 2-12 µmole/plate was observed in TA1530. Since this exposure technique does not completely accommodate the volatility of ethylene dibromide, it is probable that mutation frequencies observed (e.g., 300-1500 revs/plate over the dose range tested in strain TA1530) may be lower than could have been expected had the bacteria been exposed to the full dose of chemical. Ethylene dibromide tested by this technique at the single 10 µl dose was reported to be inactive in S. typhimurium TA1538. Because data for only a single dose were reported and because of the inaccuracy inherent in determining the effective dose by the filter paper technique, this result is insufficient for evaluating the mutagenicity of ethylene dibromide in strain TA1538 (although inactivity in strain TA1538 might be predicted since the strain is designed to detect frameshift mutagens and ethylene dibromide is more likely to cause base-substitution mutations) (EMIC-20029).

Ethylene dibromide has also been reported to be more toxic to DNA repair deficient E. coli W3478 (pol A^-) than to repair competent E. coli W3110 (pol A^+). Greater toxicity to strain P3478 may reflect potential for inducing DNA damage. The data reported are insufficient for evaluating the effect of the chemical since results at only a single dose (10 µl/plate) are presented (EMIC-20029. The adequacy of this assay as a quantitative test has been questioned by other investigators (Fluck *et al.*, 1976, EMIC-24127) because of the instability of the pol A mutant, and because of difficulties in obtaining dose-response and in demonstrating reproducibility.

Ethylene dibromide has been shown to cause forward mutations (at the *ad-3* gene locus) to a requirement for adenine in *Neurospora crassa*. The conidia were treated for 3 hours with 1.2-1.63 μl/ml ethylene dibromide in 0.06M phosphate buffer pH 7.0 containing 10% DMSO. At 1.6 μl/ml the mutation frequency induced by the compound was $30/10^6$ survivors compared to $0.5/10^6$ survivors for untreated controls (10% DMSO and buffer only) (EMIC-5480, 7225).

Ethylene dibromide has been shown to be inactive in inducing deletions in the *gal-chl* gene region of *S. typhimurium* LT-2 (EMIC-20068).

2. Chromosome Damage or Rearrangement

   a. ± Mammalian Metabolizing System: -None-

   b. No Mammalian Metabolizing System:

Ethylene dibromide has been reported to be highly active in inducing mitotic gene conversion in *S. cerevisiae* D_4. Although the data reported are insufficient for evaluation of this test, primarily because data at only a single dose were presented and no details of the method used to suggest that dose-response had been established were presented, the effect reported was strongly positive. At a concentration of 0.17 mM on treatment for 27 hours, 10.8 convertants/10^5 survivors were observed at the ade_2 locus vs. 0.48 in untreated controls and 8.85 convertants/10^5 survivors were observed at the trp_5 locus vs. 0.82 in untreated controls. The results are drawn from three trials (EMIC-20762).

B. *Drosophila*:

The chemical was reported to be active in the induction of sex-linked recessive lethal mutations in *Drosophila melanogaster*. Males were given a 0.3 mM solution of the chemical orally over a three-day period, and then were mated with sets of two new females every three days to establish three broods. Although the results of only one dose level are reported, a significant increase in percent of lethals over controls was observed, particularly in the second and third broods, which correspond to effects in spermatid and spermatocyte stages of spermatogenesis (EMIC-17636).

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Ethylene dibromide was reported to cause pink somatic mutations in stamen hair cells of *Tradescantia* (mutable clones *02*, *0106*, and *4430*). An exponential dose-response was demonstrated in all three clones (*EMIC*--21925). Similar results have been reported in several other studies (*EMIC*-18021, 18022, 18929, 18937, 21245, 23972) including one using [^{3}H] EDB (*EMIC*-23973). In one study, the mutation frequency was found to increase nearly linearly with the product of concentration and time (*EMIC*-21244). It was suggested that the phenotypic changes are associated with chromosome breakage, gene mutation, chromosome non-disjunction, or somatic crossing-over (*EMIC*-17669).

The chemical has been reported to induce chromosome aberrations and single-strand breaks in DNA in barley kernels (*EMIC*-19016).

Ethylene dibromide was reported to be inactive in inducing chromosome breaks in root tips of *Allium*, but the report is a meeting abstract and no experimental details or data were presented (*EMIC*-20037).

The combined effect of ethylene dibromide and X-rays in inducing gene damage in *Drosophila* was reported to have been studied. The report was a meeting abstract and neither the assay systems nor experimental data were presented (*EMIC*-12223).

In two review articles published in 1976 and an editorial review published in 1971, mutagenicity test results in ethylene dibromide were covered briefly (*EMIC*-11767, 23118, 23154).

V. Peripheral Literature Cited in the EMIC Data Base: (*EMIC*-4414, 6861, 7931, 8212, 14020, 15901, 19337).

June 1977

MUTAGENICITY EVALUATION

SUMMARY SHEET

Classification:
Positive _____
Negative/Inadequate X

COMPOUND: ETHYLENE GLYCOL

CAS NO.: 107-21-1

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	Ethylene glycol was demonstrated to be inactive in inducing reversions to histidine prototrophy in *Salmonella typhimurium* strains TA1535, TA1537, TA100, and TA98 both in the presence and absence of a mammalian metabolic activation system containing a rat liver microsome fraction.
Other Tests Not Reviewed:	None

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-
2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System: -None-
2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. ± Mammalian Metabolizing System:

Incorporated directly into molten agar containing the bacteria, ethylene glycol has been demonstrated to be inactive in inducing reversions to histidine prototrophy in *S. typhimurium* strains TA1535, TA1537, TA100, and TA98, both in the presence and absence of a microsome fraction (S-9) from the livers of rats pretreated with Aroclor 1254. The compound was tested at doses presumably ranging from $10-10^4$ μg/plate (EMIC-21337).

b. No Mammalian Metabolizing System: -None-

2. Chromosome Damage or Rearrangement

a. ± Mammalian Metabolizing System: -None-
b. No Mammalian Metabolizing System: -None-

B. *Drosophila*: -None-

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Evaluated: -None-

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-6010, 10798, 11001, 13043, 13098, 13911, 16090, 16515, 19026, 19340)

June 1977

Classification:
Positive ____
Negative/Inadequate X

MUTAGENICITY EVALUATION

SUMMARY SHEET

COMPOUND: PHENOL

CAS NO.: 108-95-2

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	Phenol was reported to be active in inducing reversions to streptomycin independence in *Escherichia coli* B/r Sd-4 and inactive in inducing reversions to adenine prototrophy in *Neurospora crassa* strain 70007-38701. The data reported for these tests were insufficient for establishing the results presented. A study in which the chemical was reported to be mutagenic in *Drosophila* was cited, but no data were presented on which to base an evaluation.
Other Tests Not Reviewed:	Phenol was reported to inhibit DNA repair synthesis in human diploid fibroblasts pretreated with N-acetoxy-2-acetylaminofluorene and to induce chromosome breakage in root tip cells from *Allium cepa*.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-
2. Chromosome Damage or Rearrangement in a)Germ Cells and b) Somatic Cells: -None-

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-
2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System:

When incubated with a suspension of 2-3 x 10^9 bacteria in distilled water for 12 or 24 hours, phenol (10% dose) was observed to induce reversions to streptomycin independence in *E. coli* B/r Sd-4. The data presented are insufficient for evaluation of this test as positive, since a dose-response relationship was not demonstrated in the results reported. Also, since the toxicity was high at the 10% concentration after both 12 and 24 hours of incubation (only 1.7 and 1.1% survival, respectively), the relatively high mutation frequencies may be artifactual (*EMIC*-6911; see also *EMIC*-4883 and 6912).

Phenol was reported to be inactive in inducing reversions to adenine prototrophy in *Neurospora crassa* strain 70007-38701 when mixed with a suspension of conidia in water at a concentration of 0.077M and incubated at 25°C for 30 minutes. The data reported are insufficient for establishing inactivity, primarily because results at only a single dose were presented and toxicity at the tested dose was high (87% mortality) (*EMIC*-9487).

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-
b. No Mammalian Metabolizing System: -None-

B. *Drosophila*:

A study in which phenol was reported to be mutagenic in *Drosophila* was cited in two of the literature reports monitored. No relevant data were presented (*EMIC*-4833, 10651; see also Hadorn, E. and Niggli, H., *Nature* *157*, 162-3, 1946).

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Phenol was reported to inhibit DNA repair synthesis in human diploid fibroblasts damaged by treatment with N-acetoxy-2-acetylaminofluorene (*EMIC*-20141).

Chromosome fragments were reported to have been observed in growing root tip meristems of Allium cepa treated with phenol at concentrations ranging from 0.005 to 0.02M (EMIC-10651, 10652).

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-6983, 10817, 10859, 10947, 11198, 12940, 20657, 20770, 22741, 22793).

June 1977

MUTAGENICITY EVALUATION

SUMMARY SHEET

Classification:
Positive _____
Negative/Inadequate X

COMPOUND: HYDROQUINONE (para)

CAS NO.: 123-31-9

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	Hydroquinone was reported to be more toxic to DNA repair deficient *Escherichia coli* P3478 than to repair competent *E. coli* W3110. Greater toxicity to strain P3478 may indicate potential for inducing DNA damage. No data were reported on which to base an evaluation of this test.
Other Tests Not Reviewed:	Hydroquinone has been reported to be inactive in inducing penicillin and streptomycin resistance in *Micrococcus pyogenes*. Chromosome aberrations have been observed in various types of cells from *Allium sativum* and *Vicia faba*, in roots of *Allium cepa*, in germinating seeds of *Nigella sativa* and *Trigonella foenum-graecum*, in *Chara zeylanica*, and in nodal roots of *Callisia fragrans* treated with hydroquinone. Also, studies in which hydroquinone was inactive in inducing chromosome aberrations in *Vicia faba* and in onion rootlets have been reported.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-
2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-
2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System:

It has been reported that hydroquinone is more toxic to DNA repair deficient *Escherichia coli* P3478 (Pol A$^-$) than to repair competent *E. coli* W3110 (Pol A$^+$), indicating that the chemical may induce DNA damage. This test is not readily evaluated from the data reported since no information such as doses tested, the measure of growth inhibition used, the method of exposing the bacteria to the chemical, or control results were presented (EMIC-21260).

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-
b. No Mammalian Metabolizing System: -None-

B. *Drosophila*: -None-

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Hydroquinone was reported to be inactive in inducing streptomycin and penicillin resistance in *Micrococcus pyogenes* var. *aureus* FDA209. These tests were not reviewed because the mutational events being monitored were not characterized adequately (EMIC-11162).

In several studies chromosome aberrations have been observed in plant systems treated with hydroquinone. Chromosome breaks occurred in *Allium sativum* and *Vicia faba* cells treated *in vitro* with 0.1 - 10 mM para-hydroquinone (EMIC-12235). On treatment with hydroquinone ($5 \times 10^{-5} - 1 \times 10^{-2}$M), chromosome fragments were seen in roots of *Allium cepa* (EMIC-10651, 10652). Bulbs of *Allium sativum* and germinating seeds of *Vicia faba*, *Nigella sativa*, and *Trigonella foenum-graecum* developed chromosome breaks on treatment with hydroquinone at concentrations of 0.001 to 0.1M, and the effects observed were sensitive to the presence of oxygen, decreasing when it was withdrawn (EMIC-11275).

Hydroquinone administered at 0.001, 0.005 and 0.05M for 3 hours was found to induce chromosome aberrations (bridges and fragmentation) in the lower plant *Chara zeylanica* (EMIC-16576). Effects observed in the chromosomes of nodal roots of *Callisia fragrans* treated in 0.001 - 0.5% aqueous solutions of hydroquinone included formation of "sticky bridges" and fragmentation (EMIC-17242).

In two other studies, no significant effects on plant chromosomes were observed after treatment with hydroquinone. No chromosome breaks were observed in root tip meristems of *Vicia faba* (EMIC-9488) and no visible chromosome aberrations were observed in onion rootlets treated with 5 x 10^{-3}M hydroquinone for 15 months (EMIC-6192).

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-4616, 9584, 10936, 12602, 12940, 14375, 14542).

June 1977

Classification:

Positive ____

Negative/Inadequate _X_

MUTAGENICITY EVALUATION
SUMMARY SHEET

COMPOUND: ACRYLONITRILE

CAS NO.: 107-13-1

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	Acrylonitrile has been reported to be inactive in induction of sex-linked recessive lethal mutations (Muller -5 Test) in *Drosophila melanogaster*. The data presented are inadequate for evaluation.
Other Tests Not Reviewed:	The chemical has been reported to be inactive in inducing chromosome aberrations in root tips of *Vicia faba*.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-
2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-
2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

   a. ± Mammalian Metabolizing System: -None-
   b. No Mammalian Metabolizing System: -None-

2. Chromosome Damage or Rearrangement

   a. ± Mammalian Metabolizing System: -None-
   b. No Mammalian Metabolizing System: -None-

B. *Drosophila*:

Acrylonitrile was tested for induction of sex-linked recessive lethal mutations (Muller -5 Test) in *Drosophila melanogaster*. The compound was administered by intraabdominal injection at a dose of 0.2 µl of a 0.1% solution. The authors judged the percentage of recessive lethals observed to be within control limits, but the data presented are not adequate for evaluation of the test (e.g., no evidence that the compound was tested at more than one dose level was reported, and a relatively low number of chromosomes were tested (572 in Brood I, 725 in Brood II)). The authors also suggested that a test in *Drosophila* may be inappropriate for a compound with insecticidal activity such as acrylonitrile (*EMIC*-6618).

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Acrylonitrile has been reported to be inactive both in inducing chromosome aberrations (*EMIC*-9488) and in potentiating the induction of chromosome aberrations in the presence of light and acridine orange (*EMIC*-8323) in root tips of *Vicia faba*.

V. Peripheral Literature Cited in the EMIC Data Base: (*EMIC*-4616).

June 1977

Classification:
Positive ____
Negative/Inadequate X

MUTAGENICITY EVALUATION

SUMMARY SHEET

COMPOUND: DIOXANE

CAS NO.: 123-91-1

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	None
Other Tests Not Reviewed:	Dioxane has been reported to induce mutations in barley and to enhance the mutagenicity of N-nitrosoalkylureas in wheat seeds. No effect of dioxane was observed in giant chromosomes from Chiromus plumosus. Dioxane did not induce mitotic aberrations in onion root tips.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. In vivo Treatment with Test Compound

1. Induction of Point Mutations: -None-
2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

B. In vitro Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-
2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations
   - a. ± Mammalian Metabolizing System: -None-
   - b. No Mammalian Metabolizing System: -None-
2. Chromosome Damage or Rearrangement
   - a. ± Mammalian Metabolizing System: -None-
   - b. No Mammalian Metabolizing System: -None-

B. *Drosophila*: -None-

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

p-Dioxane has been reported to induce chlorophyll mutations in treated barley seeds (*EMIC*-6917) and to enhance the mutagenicity of N-nitrosoalkylureas in wheat seeds when substituted for buffer during treatment (*EMIC*-19071).

Dioxane had little effect on the morphology and fluorescence spectrum of giant chromosomes from the salivary glands of *Chiromomus plumosus* (*EMIC*-14210) and did not induce multipolar mitosis in *Allium* root tip cells (*EMIC*-10843).

V. Peripheral Literature Cited in the EMIC Data Base: (*EMIC*-16090).

June 1977

Classification:

Positive ____

Negative/Inadequate X

MUTAGENICITY EVALUATION
SUMMARY SHEET

COMPOUND: BUTYLATED HYDROXYTOLUENE (BHT)

CAS NO.: 128-37-0

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	Administered by gavage, BHT was found to be inactive in inducing dominant lethal mutations in the rat. The chemical was also reported to be inactive in inducing dominant lethal mutations in the mouse when administered intraperitoneally, but data reported are insufficient for establishing a negative result. In addition, intraperitoneal administration may not be a relevant exposure to consider in estimating potential for genetic damage in humans. Oral administration may be a more appropriate route for BHT.

BHT was found to be inactive in inducing chromosome aberrations in bone marrow cells from rats treated by gavage. The cells were analyzed in metaphase. The chemical was likewise reported to be inactive in inducing chromosome aberrations in liver parenchymal cells from male, LAF_1 mice fed a diet containing BHT. These cells were analyzed in anaphase, and the data presented were inadequate for establishing a negative result.

In contrast, in two studies *in vitro*, increased incidences of chromosome aberrations over those in untreated controls were reported to have been observed in mammalian cells. In one study, human lung fibroblasts (WI-38) were treated in culture with BHT, and in the other study, human blood lymphocytes were treated. The data reported from both studies were inadequate for establishing activity, primarily because dose-response was not demonstrated.

BHT was found to be inactive in host-mediated assays in mice using *Salmonella typhimurium* TA1530 (reversion to histidine prototrophy) and *Saccharomyces cerevisiae* D_3 (mitotic recombination at an adenine locus) as indicator organisms. The chemical was administered by gavage and the microorganisms were incubated in the peritoneal cavity of the mice.

BHT was reported to be inactive in inducing reversions to streptomycin independence in *Escherichia coli* Sd-4-73 and in inducing sex-linked recessive lethal mutations in *Drosophila melanogaster*. No data were presented on which to base evaluations of these tests.

Other Tests Not Reviewed:

BHT has been reported to potentiate the activity of *gamma* radiation in inducing sex-linked recessive lethal mutations in *Drosophila melanogaster*, but has also been reported to reduce mutagenic effects of other agents in the following systems: 1) induction of dominant lethal mutations and heritable translocations by ethylmethanesulfonate (EMS) and other alkylating agents in mice, 2) induction of chromosome aberrations in human blood leukocytes treated in culture with 7,12-dimethylbenz(a)anthracene, 3) induction of reversions to histidine prototrophy in *S. typhimurium* TA1950 and TA1952 treated with safrole or a urinary metabolite of safrole and in five strains of *S. typhimurium* treated with some anthraquinones, and 4) induction of sex-linked recessive lethal mutations in *Drosophila* fed EMS. No effect on the induction of dominant lethal mutations or heritable translocations by X-ray was observed in mice. Also, no effect on the induction of translocations by EMS was observed in one study in which mice were fed a diet containing BHT for 30 days.

The chemical was also reported to be inactive and slightly antimutagenic in inducing chromosome aberrations in root tip cells from *Allium fistulosum*, to reduce the incidence of chromosome aberrations induced by gamma radiation and ethyleneimines in germinating seeds from *Crepis capillaris*, and to induce polyploidy and mitotic disturbances in the *Crepis capillaris* system.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-

2. Chromosome Damage or Rearrangement in

a. Germ Cells:

BHT was found to be inactive in inducing dominant lethal mutations in the rat. In this test, the chemical was administered by stomach tube in single doses of 30, 900, or 1400 mg/kg or in multiple doses of 30, 250, or 500 mg/kg to groups of 10 male rats. The treated males were mated for 8 weeks to two virgin females per week, and the pregnant females were autopsied for analysis in mid-gestation. No statistically significant responses indicative of dominant lethals were observed in the parameters monitored (e.g., dead implants/pregnant female, dead implants/total implants, corpora lutea/pregnant female) in the females from any of the mating weeks (EMIC-17284; see also EMIC-20877).

The chemical was also reported to be inactive in inducing dominant lethal mutations in the mouse. In this test, groups of 7 - 9 male, ICR/HA Swiss mice were given single doses of 250, 500, 1000, or 2000 mg/kg by intraperitoneal injection. The treated males were mated for 8 weeks to three virgin females per week and pregnant females were autopsied for analysis 13 days after midweek of mating. The data presented are insufficient for evaluation of this test. For example, none of the parameters used to detect dominant lethals (e.g., early fetal deaths/pregnant female and total implants) were tabulated. Also, the effects observed after intraperitoneal injection may not be relevant to effects observed in humans exposed to the chemical. Oral administration may have been a more appropriate route of exposure (EMIC-12984).

b. Somatic Cells:

BHT was found to be inactive in inducing chromosome aberrations in bone marrow from treated rats. In this test, groups of 15 rats were given single doses of 30, 900, or 1400 mg/kg by stomach tube, and bone marrow was sampled from five rats at each dose level at 6, 24, and 48 hours after treatment. Three additional groups of five rats were given multiple doses of 30, 250, and 500 mg/kg, and bone marrow was sampled after treatment ended. A total of 250 metaphase cells (5 rats x 50 cells/rat) was monitored at each dosage level and treatment time. No significant increase in the incidence of chromosome aberrations over that in untreated controls was observed in any sample (EMIC-17284; see also EMIC-20877).

BHT was also reported to be inactive in inducing chromosome aberrations in liver parenchymal cells from male, LAF_1 mice fed a diet containing 0.5% BHT from weaning to age 21 months. Seventy hours before sacrifice and analysis, the mice were dosed with CCl_4 to induce liver regeneration. The cells were analyzed in anaphase. The data presented were insufficient for establishing a negative result, because results at only a single dose were reported, the number of cells monitored was not specified, and only five animals were tested (EMIC-8869).

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System:

An increased incidence of chromosome aberrations over that in untreated controls was observed in human lung fibroblasts (WI-38) grown in the presence of 2.5, 25, and 250 μg/ml BHT during the last 24 hours of cultivation. The incidences of cells with aberrations were 28.1% (of 267 cells), 17.5% (of 280 cells), and 20% (of 50 cells) with increasing dose. Cells were analyzed in anaphase; the predominant aberration detected at all three dose levels was acentric fragments; and the effects observed were comparable to those in cells treated by the same method with triethylenemelamine (TEM). The data presented are inadequate for establishing the results as positive evidence of a gene-damaging effect of BHT, primarily because dose response was not demonstrated (EMIC-17284).

BHT at 40 μg/ml was also reported to be active in inducing chromosome aberrations (breaks) in human lymphocytes treated *in vivo* for 24 hours and analyzed in metaphase. The data presented are inadequate for establishing a positive effect of BHT because dose response was not demonstrated (the chemical was tested over the dose range of 5 - 50 μg/ml). Also, the experimental method was not clearly defined (e.g., the method of determining the mitotic index was unusual and not defined, and the sample sizes and cell populations treated were not recorded) (EMIC-17100).

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally:

BHT was found to be inactive in host-mediated assays in the mouse using *Salmonella typhimurium* TA1530 and *Saccharomyces cerevisiae* D_3 as indicator organisms. Reversion to histidine prototrophy was the mutational event monitored in *Salmonella* and mitotic recombination at the *ade*$_2$ locus was the genetic event monitored in the *Saccharomyces*. The chemical was administered to groups of 8 mice by stomach tube in single doses of 30, 900, or 1400 mg/kg or in multiple doses of 30, 250, or 500 mg/kg. No significant increase in the incidences of mutants over those in untreated controls were observed in either the Salmonella or the Saccharomyces. The chemical was also reported to be inactive in vitro in both microorganisms, but no data were presented (EMIC-17284).

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System:

BHT, applied to a filter paper disc which was then laid on nutrient agar containing the bacteria, was reported to be inactive in inducing reversions to streptomycin independence in Escherichia coli Sd-4-73. This report is essentially a review article and no other data are presented on which to base an evaluation (EMIC-5412).

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-
b. No Mammalian Metabolizing System: -None-

B. Drosophila:

BHT was reported to be inactive in inducing sex-linked recessive lethal mutations in Drosophila melanogaster. This report is a meeting abstract and no data are reported on which to base an evaluation of this test (EMIC-14078).

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

BHT has been reported to potentiate the activity of gamma radiation in inducing sex-linked recessive lethal mutations in Drosophila melanogaster (EMIC-16210, 14078).

The chemical has also been reported to reduce mutagenic effects of other agents in various systems. When fed to mice it reduced the frequency of dominant lethal mutations and heritable translocations induced by treatment with EMS and other (not specified) monofunctional alkylating agents, but not those induced by X-rays (EMIC-7504). Fewer chromosome breaks were seen in human leukocytes treated in culture with 7,12-dimethylbenz(a)-anthracene (DMBA) and with BHT than with DMBA alone (EMIC-16572, 18922, 19650). Drosophila melanogaster fed a diet containing

2 mg/g BHT were reported to be less susceptible to the induction of sex-linked recessive lethal mutations by EMS than Drosophila not fed with BHT (cf. Drosophila treated with X-rays which did not show decreased susceptibility with BHT) (EMIC-20887). In the presence of a mammalian metabolic activation system containing a microsome fraction from the livers of animals prefed BHT for 12 days, the activities of safrole and a urinary metabolite of safrole in inducing reversions to histidine prototrophy in *Salmonella typhimurium* strains TA1950 and TA1952 were significantly reduced (EMIC-9525). Also, in tests of some anthraquinones (not specified) the mutagenic activities in five histidine-requiring strains of *S. typhimurium* (not specified) were reported to be reduced substantially when incubations were carried out in the presence of BHT (EMIC-23948).

No significant effect on the induction of translocations was seen in mice treated with 250 mg/kg EMS after feeding on a diet containing BHT for 30 days (EMIC-9284, 17001).

BHT was reported to be inactive in inducing chromosome aberrations and to be slightly anti-mutagenic in root tip meristem cells from *Allium fistulosum*. The aberration frequency decreased from 6.48 to 2.43% on treatment of the root tips with a 1:1 saturated aqueous solution of BHT (EMIC-5004). The chemical was reported to decrease the incidence of chromosome aberrations induced by gamma radiation and ethyleneimines in germinating seeds of *Crepis capillaris* (EMIC-20850), but it was also reported to induce polyploidy (0.01% of the cells treated) and mitotic disturbances in the same system (EMIC-16076).

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-10641, 11163, 14858, 15901, 16214, 16247, 18167, 19646, 21823, 21941, 23142).

June 1977

MUTAGENICITY EVALUATION
SUMMARY SHEET

Classification:
Positive _____
Negative/Inadequate X

COMPOUND: THIRAM

CAS NO.: 137-26-8

SUMMARY EVALUATION:

Positive Tests Reviewed: None

Negative/Inadequate Tests Reviewed:

Thiram, administered in drinking water for six months, was reported to be inactive in inducing dominant lethal mutations in rats. The data presented were insufficient for establishing inactivity.

The chemical was reported to be active in inducing chromosome aberrations in mouse bone-marrow cells after oral or intraperitoneal administration. The data presented are insufficient for evaluation of these tests.

Thiram, after incubation with nitrite at pH 1, was reported to be active in inducing mutations (not specified) in *Escherichia coli* K-12 in the presence of a mammalian metabolic activation system containing liver microsomes. No data were presented on which to base an evaluation of this test.

The chemical was reported to be inactive in inducing reversions to tryptophan prototrophy in qualitative tests in *E. coli* WP-2 hcr$^-$ and *E. coli* WP-2 hcr$^+$ and in inducing reversions to methionine prototrophy in *Saccharomyces cerevisiae* strain 632/4. For these tests, the data presented were inadequate for evaluation.

The chemical was reported to be slightly toxic to *Bacillus subtilis* M45 (rec$^-$) and not toxic to *B. subtilis* H17 (rec$^+$). Greater toxicity to DNA repair deficient M45 than to repair competent H17 may be indicative of potential for inducing DNA damage. The data reported are insufficient for evaluation of the results.

Other Tests Not Reviewed: Thiram was reported to induce two distinct variants in the fungus *Alternaria mali*. The mutational events occurring in the production of these variants were not characterized. The chemical was also reported to induce chromosomal aberrations in barley seeds and morphological and chlorophyll mutants in wheat.

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-

2. Chromosome Damage or Rearrangement in

a) Germ Cells:

Thiram, at a dose level of 10 mg/ml in drinking water administered *ad lib* for six months, was reported to be inactive in inducing dominant lethal mutations in male rats. Dominant lethals were monitored at the end of treatment and 2-1/2 months after treatment ended (8-1/2 months after initiation of the experiment). The data reported were insufficient for establishing inactivity. For example, the parameters monitored (e.g., early fetal deaths, total implants) were not tabulated, the mating and autopsy schedules were not described, and results at only a single dose were presented (EMIC-23235).

b) Somatic Cells:

Thiram was reported to induce significant incidences of chromosome aberrations in mouse bone marrow cells on administration of 100 or 1000 mg/kg by stomach tube. The incidences were, respectively, 3.9 and 7.83% of metaphase cells analyzed at 24 hours after treatment. A higher aberration frequency (9.5%) was found on intraperitoneal administration of 100 mg/kg. The data presented were insufficient for evaluation of these tests, primarily because the experimental methods were not adequately described and the results are reported as total aberrations rather than being listed by type (EMIC-17423; see also EMIC-22480).

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System:

Thiram which had been incubated with nitrite at pH 1 was reported to induce mutations in *Escherichia coli* K-12 (strain not specified, but presumably 343/113) in the presence of a mammalian metabolic activation system containing liver microsomes. This report is a meeting abstract, and no data are presented on which to base an evaluation of the test. Dimethylnitrosamine was detected analytically in the thiram which had been incubated with nitrite (EMIC-22329).

b. No Mammalian Metabolizing System:

Thiram (85%), at single doses of approximately 1-3 mg applied to a filter paper disc and laid on agar containing 10^8 bacteria, was reported to be inactive in inducing reversions to tryptophan prototrophy in *Escherichia coli* WP-2 hcr$^+$ and in *E. coli* WP-2 hcr$^-$. The data presented were insufficient for evaluation because these were qualitative tests and results at only single doses were reported. Also, thiram is insoluble in water and it was not clear that the chemical was able to diffuse through the agar to reach the bacteria by the method used (EMIC-21799).

Thiram was reported to be inactive in inducing reversions to methionine prototrophy in *Saccharomyces cerevisiae* strain 632/4. Apparently, the compound was tested at several doses applied in aqueous suspension to a filter paper disc which was laid on agar containing the yeast. No other data were provided on which to base an evaluation of this test. In particular, it was not clear that the thiram was able to penetrate the agar and reach the yeast (EMIC-24000).

2. Chromosome Damage or Rearrangement

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System:

At a single dose of 2.0 μg/plate applied to a filter paper disc which was then laid on agar containing the bacteria, thiram (in DMSO) was reported to be slightly toxic to Bacillus subtilis M45 (rec^-) and not toxic to B. subtilis H17 (rec^+). Greater toxicity to M45 than to H17 may be indicative of potential for inducing DNA damage, but the effect of thiram was judged to be insignificant because the length of the zone of growth inhibition (the measure of toxicity used) observed was only 2.0 mm. Several doses were tested and the results reported are those at the dose at which minimal inhibition of H17 and reproducible growth inhibition of M45 were elicited. It is not clear that these results represented the maximum toxicity differential obtained. The low toxicity in M45 and the lack of toxicity in H17 may indicate that the chemical did not adequately penetrate the agar to reach the bacteria. The data presented are insufficient for establishing inactivity (EMIC-21385; see also EMIC-22827).

B. Drosophila: None

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Thiram was reported to induce two distinct variants in the fungus Alternaria mali. These data were not reviewed because the mutational events occurring were not adequately characterized (EMIC-15108, 17214).

Chromosome abnormalities were observed in barley seeds germinated for 5-10 days in the presence of 250-500 ppm thiram (EMIC-8085; see also EMIC-20691). Thiram was also reported to induce morphological and chlorophyll mutants in progeny of spring wheat plants treated with the fungicide at concentrations of 100 kg/ton, but no significant chromosome aberrations were observed in plants from wheat seeds treated at a concentration of 0.5-200 kg/ton (EMIC-19513; see also EMIC-18843).

Mutagenicity data on thiram were covered briefly in a review article published in 1976 (EMIC-22480).

V. Peripheral Literature Cited in the EMIC-12316, 21606).

June 1977

MUTAGENICITY EVALUATION
SUMMARY SHEET

Classification:
Positive ____
Negative/Inadequate X[1]

COMPOUND: ZIRAM

CAS NO.: 137-30-4

SUMMARY EVALUATION:

Positive Tests Reviewed:

Ziram was shown to induce a dose-related increase in the incidence of chromosome and chromatid breaks in human lymphocytes treated *in vitro* at concentrations ranging from 0.0006 to 0.06 μg/ml.

Negative/Inadequate Tests Reviewed:

Administered by gavage at a dose of 100 mg/kg, ziram was reported to induce an increased incidence of chromosome aberrations over that in untreated controls in bone marrow cells of treated mice. The data presented are inadequate for establishing activity.

A significant increase in chromosome and chromatid breaks over that in untreated controls was observed in leukocytes of nine workers exposed to ziram over 3 - 5 years. Unfortunately, the sample size and other data reported are inadequate for eliminating other possible causes.

Ziram was reported to be inactive in inducing forward mutations to streptomycin resistance in *Escherichia coli*, mutation to ability to metabolize galactose in *E. coli* K-12 (*galR*^{s}), reversion to prototrophy in two leucine-requiring strains of *Serratia marcescens* (strains A21 and A742), forward mutation to 5-methyltryptophan resistance in *E. coli*, mitotic gene conversion in *Saccharomyces cerevisiae* (presumably strain D_4), and reversions to methionine prototrophy in

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[1] The reviewers judged that the one adequate positive test in human lymphocytes was not sufficient for establishing ziram as a mutagen. The reasons are that (a) chromosome damage observed *in vitro* may not be a clear cut demonstration of a chemical effect (e.g., physical factors, such as altered ion concentrations, may play a role), (b) the blood treated may have been a biased sample and (c) because of the subjectivity of scoring chromosome aberrations, confirmation by a second group of investigators would have been desirable. However, in estimating the gene-damaging potential of ziram, the cytogenetic effects observed by this one group of investigators in exposed workers and in treated mice, as well as those in human blood *in vitro* should not be ignored.

Saccharomyces cerevisiae 632/4. The data presented are insufficient for evaluation of these tests. In another study, ziram was demonstrated to be inactive in inducing mitotic gene conversion in Saccharomyces cerevisiae D_4.

The chemical was reported to be slightly more toxic to DNA repair deficient Bacillus subtilis M45 than to repair competent B. subtilis H17. Greater toxicity to M45 may be indicative of potential for inducing DNA damage. The test was judged by the investigators to be negative, but the data presented are inadequate for evaluation.

Ziram was reported to be inactive in inducing sex-linked recessive lethal mutations in Drosophila melanogaster. The data reported are insufficient for establishing inactivity.

Other Tests Not Reviewed: Ziram was reported to induce chromosome abnormalities in barley seeds.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian System

A. In vivo Treatment with Test Compound

1. Induction of Point Mutations: -None-

2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells

Ziram, administered to mice by gavage at a dose of 100 mg/kg, was reported to induce an incidence of chromosome aberrations in bone marrow cells greater than that observed in untreated controls (3.13% vs. 0.46% - 0.73% in untreated controls). The cells were analyzed in metaphase 24 hours after treatment. The data presented are not sufficient for evaluation of the test because results at only a single dose are reported, the experimental methods are not adequately documented, and the results are reported as total aberrations rather than being listed by type (EMIC-17423; see also EMIC-22480).

A significant increase in chromosome and chromatid breaks over that in unexposed controls was observed in peripheral leukocytes from workers employed in handling or packing ziram over a period of three to five years. These results are presented because the increased incidences of aberrations were significant for each of the nine workers studied, but evaluation is not feasible because the data reported and the sample size are inadequate for eliminating other possible causes (EMIC-7849; see also EMIC-12482).

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-

2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System):

Ziram was shown to induce a dose-related incidence of chromosome and chromatid breaks in human lymphocytes treated *in vitro* at concentrations ranging from 0.0006 to 0.06 µg/ml. The ziram was dissolved in acetone, and the cells were treated for 50-53 hours and then analyzed in metaphase. The incidences of breaks were significantly greater than untreated and acetone controls at all but the lowest concentration. There was limited evidence of nonrandom distribution of breaks. That is, a significantly higher percentage of breaks than expected by random distribution was observed in chromosome 2 (EMIC-10968).

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations

a. +/- Mammalian Metabolizing System: -None-

b. No Mammalian Metabolizing System:

Ziram was reported to be inactive in inducing reversions to methionine prototrophy in *Saccharomyces cerevisiae* strain 632/4. Apparently, the compound was tested at several doses applied in aqueous suspension to a filter paper disc which was laid on agar containing the yeast. No other data were provided on which to base an evaluation of this test. In particular, it is not clear that the chemical was able to penetrate the agar and reach the yeast (EMIC-24000).

Ziram has been reported to be inactive in inducing forward mutations to streptomycin resistance in *Escherichia coli*, mutation to ability to metabolize galactose in a strain of *E. coli* K-12 (carrying the galR^s gene), reversion to prototrophy in two leucine-requiring strains of *Serratia marcescens* (strains A21 and A742), and forward mutation to 5-methyltryptophan resistance in *E. coli*. No data were given on which to base evaluations of these tests (EMIC-20762).

At a single dose of 0.6 µg/plate, applied to a filter paper disc which was then laid on the agar containing the bacteria, ziram (in DMSO) was reported to be slightly more toxic to DNA repair deficient *B. subtilis* M45 (rec$^-$) than to repair competent *B. subtilis* H17 (rec$^+$), but the effect was judged to be insignificant since a difference in the lengths of the zones of growth inhibition (the measure of toxicity used) of only 1.0 mm was observed. Greater toxicity to M45 may be indicative of potential for inducing DNA damage. The data reported are insufficient for use in evaluating this test, primarily because results at only a single dose were presented and the toxicities observed to both strains of *B. subtilis* were very low. Other doses were tested and the results at the dose eliciting minimal inhibition of H17 and reproducible growth inhibition of M45 were reported, but is not clear that these results represented the maximal toxicity differential obtained. The lengths of the zones of inhibition of growth were 1.5 mm in M45 and 0.5 mm in H17. These values are low enough that there is no certainty that the chemical reached the bacteria (EMIC-21385; see also EMIC-22827).

2. Chromosome Damage or Rearrangement

   a. +/- Mammalian Metabolizing System: -None-

   b. No Mammalian Metabolizing System:

Ziram, tested as the commercial preparation Fuschin-Ultra, was demonstrated to be inactive in inducing mitotic gene conversion in *Saccharomyces cerevisiae* D_4 when incubated with the yeast in phosphate buffer (pH 7.5) for four hours at 25°C. The chemical was tested at several concentrations for induction of conversions both to adenine (*ade_2* locus) and to tryptophan (*trp_5* locus) prototrophy. At the optimal concentrations tested (maximum number of convertants observed) at both loci, the activities observed were not significantly greater than those of untreated controls. That is, at 500 ppm the conversion frequency at the *ade_2* locus was $17.8/10^6$ survivors compared to $12.5/10^6$ survivors for the untreated control, and at 1000 ppm the conversion frequency at *trp_5* was $14.7/10^6$ survivors compared to $7.3/10^6$ survivors for the untreated control (EMIC-7717).

In a second study, the chemical was observed to be inactive in inducing mitotic gene conversion in *Saccharomyces cerevisiae* (presumably strain D_4). No data were presented on which to base an evaluation of this test (EMIC-20762).

B. *Drosophila*:

Ziram was reported to be inactive in inducing sex-linked recessive lethal mutations in postmeiotic stages of spermatogenesis in *Drosophila melanogaster* (Muller-5 Test) when administered in a single dose of 0.2 µl of a 0.015% aqueous suspension. The data presented are insufficient for establishing inactivity, primarily because results at only a single dose are reported and the number of chromosomes tested appears to be low (only 378 chromosomes were tested in the treated *Drosophilia* vs. 41921 in the untreated controls and approximately 600 in *Drosophila* treated with other chemicals in the same study) (EMIC-6618).

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

Chromosome abnormalities were observed in barley seeds germinated for 5 - 10 days in the presence of 250 - 500 ppm ziram (EMIC-8085; see also EMIC-20691).

Mutagenicity data on ziram were covered briefly in a review article published in 1976 (EMIC-22480).

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-12481).

June 1977

MUTAGENICITY EVALUATION

SUMMARY SHEET

Classification:

Positive ____

Negative/Inadequate X

COMPOUND: 2-AMINOETHANOL

CAS NO.: 141-43-5

SUMMARY EVALUATION:

Positive Tests Reviewed:	None
Negative/Inadequate Tests Reviewed:	None
Other Tests Not Reviewed:	2-Aminoethanol was reported to be inactive in inducing mutations to phage and streptomycin resistance in *Xanthomonas phaseoli* var. *fuscans* and in inducing multipolar mitoses in *Allium* roots.

Evaluation of Testing Data Reported in Literature Cited in the EMIC Data Base:

I. Mammalian Systems

A. *In vivo* Treatment with Test Compound

1. Induction of Point Mutations: -None-
2. Chromosome Damage or Rearrangement in a) Germ Cells and b) Somatic Cells: -None-

B. *In vitro* Treatment with Test Compound

1. Induction of Point Mutations (+/- Mammalian Metabolizing System): -None-
2. Chromosome Damage or Rearrangement (+/- Mammalian Metabolizing System): -None-

II. Host-Mediated Assays

A. Indicator Organism or Cell System Administered Intraperitoneally: -None-

B. Indicator Organism or Cell System Exposed to Body Fluids or Tissues of Treated Animals by Other Routes: -None-

III. Non-Mammalian Systems

A. Microbial Systems

1. Induction of Point Mutations
    - a. +/- Mammalian Metabolizing System: -None-
    - b. No Mammalian Metabolizing System: -None-
2. Chromosome Damage or Rearrangement
    - a. +/- Mammalian Metabolizing System: -None-
    - b. No Mammalian Metabolizing System: -None-

B. *Drosophila*: -None-

IV. Results of Other Tests of Genetic Damage Reported in the Literature But Not Reviewed:

2-Aminoethanol was reported to be inactive in inducing mutations to phage and streptomycin resistance in *Xanthomonas phaseoli* var. *fuscans*. The tests were not evaluated because this system has not been adequately characterized as a screen for the induction of gene damage (EMIC-11454).

The chemical was reported to be inactive in the induction of multipolar mitoses in *Allium* roots (EMIC-10843).

V. Peripheral Literature Cited in the EMIC Data Base: (EMIC-19324, 19343).

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OAK RIDGE NATIONAL LABORATORY

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DEFICIENT MUTANT OF E.COLI FOR
THE RAPID DETECTION OF CARCINOGENS
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IV. STUDY OF CHEMICALS FROM TABLE ENTITLED "POTENTIAL INDUSTRIAL CARCINOGENS AND MUTAGENS"

A. Preparation of Tables Containing Economic Information

In this part of Research Request No. 1, SRI provided selected information on a list of 72 chemicals provided by the Project Officer. These chemicals were representative of ten major classes (and numerous structural classes) which had been identified in a table prepared by Dr. Lawrence Fishbein of the National Center for Toxicological Research, Jefferson, Arkansas, as potential industrial carcinogens and mutagens. The information on these chemicals supplied by SRI included: (1) CAS numbers; (2) production data, if available; and (3) copies of any available Stage I or Stage II dossiers that had already been completed as part of the NCI project. This information was tabulated and forwarded to the Project Officer in December 1976. At the request of the Project Officer, additional information on the price and total U.S. market value of these chemicals was subsequently obtained, and forwarded in April 1977.

As stipulated in Research Request No. 1, the ten major classes identified in Dr. Fishbein's table entitled "Potential Industrial Carcinogens and Mutagens" were to be expanded to include other chemicals identified as members of the classes. Work was begun on developing an expanded list of names (and CAS numbers) for Class IA, Epoxides, using sources available at SRI. Subsequently, as an aid to this expansion, the Project Officer provided a list of 415 chemicals arranged by the major classes and structural classes and identified only by CAS number. (Although Research Request No. 1 stated that such additional data would be identified by chemical name also, SRI had to obtain names for these chemicals before further work.)

Using the CAS numbers provided, the corresponding chemical names were obtained from SRI's tape of 26,000 commercially significant chemicals produced as part of a project for the NCI. Two computer printouts were then generated and sent to the Project Officer on February 10, 1977. One printout contained the chemical names and their CAS numbers, subdivided according to the ten major classes and their structural classes. The other printout contained the chemical names ranked by CAS number in increasing order. Since the expansion of the list of chemicals in structural class IA, Epoxides, was nearly complete when the list of CAS numbers was received from the Project Officer, it was not necessary to include these epoxides in the work to establish the names of chemicals in the classes. However, for information purposes, a typed list of the CAS numbers and names for these epoxides is included as the first page of the list ordered by structural class. These printouts are reproduced in Appendix A.

Research Request No. 1 stated that a maximum of 400 chemicals would require identification of commercial significance after SRI identified additional members of each class by reviewing a variety of literature to expand the classes. However, a total of 487 chemicals were already provided by the Project Officer for this purpose. When SRI carried out this review, different sources were used for particular classes, depending on the unique sources available for the class itself. General sources included activity nodes from the NCI data base, monographs on potential carcinogens prepared by the International Agency for Research On Cancer, SRI's Directory of Chemical Producers-U.S.A., and chemical industry trade literature. The chemicals identified in the review were then assigned to the appropriate major classes and structural classes.

This review brought the number of chemicals assigned to the ten major classes to a total of 1791. SRI classified the chemicals in each major class or structural class into three categories: (1) those with annual production greater than one million pounds; (2) those with annual production greater than one thousand pounds (in some cases, this category was further divided into those chemicals for which a specific production figure was provided and those chemicals for which available information could only identify them as being produced in quantities greater than one thousand pounds annually); and (3) those chemicals with annual production less than one thousand pounds. One thousand pounds is used by the International Trade Commission as the minimum weight quantity at which production of a chemical is reported. One million pounds is commonly used as a measure of a commodity chemical. Consequently, the pound as a unit of weight has been adopted for all of the sections of this report dealing with economic aspects of the chemicals.

The ten major classes (because of the use of structural classes, a total of 26 separate categories were actually used) are presented in Table 4-1, along with the number of chemicals assigned to each major class or structural class. The column headed "Orig. Chems." shows the distribution of the original 72 chemicals provided in the "Potential Industrial Carcinogens and Mutagens" table. The next three columns show the distribution of the chemicals provided by the Project Officer and obtained from the SRI review with one column for each of the three production volume categories. (These columns exclude those chemicals already identified in the first column.) The final column represents the total number of chemicals identified in each major class or structural class.

Table 4-1

NUMBER OF CHEMICALS IN MAJOR CLASSES AND STRUCTURAL CLASSES

		Added Chemicals With Annual Production:			
	Orig. Chems.	>1 Million Pounds	>1 Thousand Pounds	<1 Thousand Pounds	Total
I. Alkylating Agents					
A. Epoxides	6	6	19	43	74
B. Lactones	1	1	27	18	47
C. Aziridines	3	0	5	7	15
D. Alkyl Sulfates	2	0	0	11	13
E. Sultones	2	0	2	0	4
F. Aryl Dialkyl Triazines	2	0	3	20	25
G. Diazoalkanes	1	0	0	5	6
H. Phosphoric Acid Esters	2	19	53	26	100
I. Halogenated Saturated Hydrocarbons	2	7	55	20	84
J. Halogenated Alkanols	2	2	8	10	22
K. Halogenated Ethers	3	2	5	10	20
L. Aldehydes	2	9	47	19	77
Subtotal	28	46	224	189	487
II. Acylating Agents	4	9	69	7	89
III. Peroxides	5	7	26	2	40
IV. Halogenated Hydrocarbons and Derivatives					
A. Halogenated Unsaturated Hydrocarbons	4	4	17	4	29
B. Halogenated Methanes	3	5	15	5	28
C. Halogenated Aryl Derivatives	1	26	38	0	65
D. Halogenated Polyaromatics	1	4	43	3	51
Subtotal	9	39	113	12	173
V. Hydrazines, Hydroxylamines and Carbamates					
A. Hydrazines	4	5	50	84	143
B. Hydroxylamines	3	1	6	13	23
C. Carbamates	1	4	32	16	53
Subtotal	8	10	88	113	219
VI. N-Nitroso Compounds	2	1	7	50	60
VII. Aromatic Amines	8	26	417	0	451
VIII. Azo Compounds	4	15	224	0	243
IX. Nitrofurans	3	0	6	9	18
X. Azides	1	0	5	5	11
Total	72	153	1179	387	1791

Several of the major class or structural class titles designated by EPA were altered for various reasons. "Alkane Halides" was changed to "Halogenated Saturated Hydrocarbons" to include compounds containing more than one carbon atom. "Halogenated Methanes" (previously titled "Halogenated Saturated Hydrocarbons") includes compounds containing only one carbon atom. "Halogenated Aryl Derivatives" is limited to compounds containing only one aromatic ring, whereas "Halogenated Polyaromatics" includes compounds containing more than one aromatic ring. "Nitrosamines" was changed to "N-Nitroso Compounds" to include other types of N-nitroso compounds. "Azo Dyes" was altered to "Azo Compounds" so as not to limit the class to just dyes.

After the chemicals in each major class/structural class were identified, information on annual production was gathered and the chemicals were assigned to the appropriate category. Additional data were then sought on the chemicals, the scope of which depended on which of the three production volume categories were involved. For the chemicals with annual production greater than one million pounds, the Project Officer requested that price and market value be included. This was in addition to the CAS number, an indication of the availability of NCI Stage I and Stage II dossiers, and production data, which were collected for both the greater-than-one-million-pound and greater-than-one-thousand-pound chemicals. Only the CAS number, if readily available, was sought for the less-than-one-thousand-pound chemicals.

The information gathered was usually compiled into three tables for each major class/structural class. However, in the preparation of the tables, emphasis was placed on identifying chemicals in the two larger volume categories. Consequently, tables were not prepared for the category of chemicals with annual production of less than one thousand pounds for: (1) Class IV C, Halogenated Aryl Derivatives, because of the extremely large number of chemicals that would fall into this category; and (2) Class VII, Aromatic Amines, and Class VIII, Azo Compounds, because of the large number of chemicals identified in the category of chemicals with annual production greater than one thousand pounds.

The tables were dated when they were sent to the Project Officer, and the dates range over the course of several months. After completion, some tables were updated with more current information and/or corrections and the revision dates were added. The final versions of the tables, with the original 72 chemicals underlined, are included in Section IV.B of this report.

At the request of the Project Officer, certain structural groups are also identified in the tables. For the structural classes IV C Halogenated Aryl Derivatives and IV D Halogenated Polyaromatics, those compounds having no other functional groups are designated by an NF in the category tables. For the major class VII Aromatic Amines, the groups identified are biphenylamines (designated by a B in the category tables), methylenebis(dianilines) (M), and naphthylamines (N).

An additional five chemicals divided into four classes — Aromatic Hydrocarbons, Cyclic Ethers, Heterocyclic Amines, and Phosphoramides — were later supplied by the Project Officer as a result of further studies by Dr. Fishbein. SRI was asked to provide annual production figures, price data, market value, and any completed Stage I and Stage II dossiers for these chemicals. (No additional information on these classes was requested, and these chemicals are not included in Table 4-1.) The tables containing data on these chemicals, which were sent to the Project Officer on April 22, 1977, are reproduced in Appendix B.

B. Preparation of Market Forecasts

As required by Research Request No. 1, market forecasts were prepared for all chemicals in the ten major classes that were identified by SRI as having annual production greater than or equal to one million pounds, excluding those chemicals which are used almost exclusively as drugs or pesticides. Whenever possible, chemicals within one major class/structural class which had very smiliar uses were discussed as a group rather than individually. The market forecasts included: (1) a discussion of production and trade statistics; (2) consumption patterns, whenever possible; (3) growth trends; (4) a brief summary of current uses as well as potential new applications; and (5) growth trends in end-market consumption. Although not specified in Research Request No. 1, a discussion of possible substitutes for each chemical was also included in the market forecasts at the request of the Project Officer.

Market forecasts were prepared for a total of 109 chemicals. These forecasts, followed by the corresponding production volume category tables for each major class/structural class shown in Table 4-1 are presented on pages 4-11 through 4-264. An alphabetical listing of the chemicals having market forecasts is presented in Table 4-2.

Table 4-2

ALPHABETICAL LISTING OF CHEMICALS HAVING MARKET FORECASTS

Acetaldehyde, 4-85
Acetic anhydride, 4-98
Acetylsulfanilyl chloride, 4-155
Acrolein, 4-87
Alkyl (predominantly C_{12} and C_{14})diglycidyl ethers, 4-13
Anisic aldehyde, 4-92
Aziridine, 4-29

Benzoyl chloride, 4-107
Benzoyl peroxide, 4-122
Benzyl chloride (see alpha-Chlorotoluene)
Bis(2-chloroethoxy)methane, 4-79
Bis(2-chloroisopropyl ether) (see Bis(2-chloro-1-methylethyl ether))
Bis(2-chloro-1-methylethyl)ether, 4-78
2-Butanone peroxide (see Methyl ethyl ketone peroxide)
Butylene oxide (see 1,2-Epoxybutane)
tert-Butyl peroxybenzoate, 4-122
tert-Butylperoxy-2-ethylhexanoate, 4-122
tert-Butyl peroxypivalate, 4-122
n-Butyraldehyde, 4-85
γ-Butyrolactone, 4-23

Carbon tetrachloride, 4-141
Chloral, 4-88
Chlorendic anhydride, 4-109
Chlorobenzene (see Monochlorobenzene)
2-Chloro-1,3-butadiene, 4-131
Chloroform, 4-145
Chloroprene (see 2-Chloro-1,3-butadiene)
1-Chloro-2-propanol (see Propylene chlorohydrins)
2-Chloro-1-propanol (see Propylene chlorohydrins)
alpha-Chlorotoluene, 4-151
Cinnamaldehyde, 4-91
Cresyl diphenyl phosphate, 4-47
Cumene hydroperoxide, 4-118

C.I. Acid Blue 9, 4-208
C.I. Acid Yellow 151, 4-236
C.I. Direct Black 38, 4-235
C.I. Direct Blue 218, 4-238
C.I. Disperse Blue 79, 4-235
C.I. Disperse Yellow 3, 4-234
C.I. Pigment Blue 19, 4-206
C.I. Pigment Red 3, 4-243
C.I. Pigment Red 48, 4-241
C.I. Pigment Red 49, barium toner, 4-239
C.I. Pigment Red 49, calcium toner, 4-239

Table 4-2
(continued)

C.I. Pigment Red 52, 4-242
C.I. Pigment Red 53, barium toner, 4-241
C.I. Pigment Red 57, calcium toner, 4-244
C.I. Pigment Yellow 12, 4-239
C.I. Pigment Yellow 14, 4-242

1,2-Dibromoethane, 4-63
2,3-Dibromo-1-propanol, 4-74
Di-tert-butyl peroxide, 4-122
ortho-Dichlorobenzene, 4-153
para-Dichlorobenzene, 4-154
3,3'-Dichlorobenzidine base and salts, 4-204
1,2-Dichloroethane, 4-59
1,1-Dichloroethylene, 4-133
Dichloroethylformal (see Bis(2-chloroethoxy)methane))
Dichloroisopropyl ether (see Bis(2-chloro-1-methylethyl ether))
Dichloromethane (see Methylene chloride)
1,2-Dichloropropane, 4-64
Diphenyl isodecyl phosphate, 4-47
Diphenyl octyl phosphate, 4-47

Endrin, 4-16
Epichlorohydrin, 4-13
Epoxidized esters, 4-14
Epoxidized linseed oil (see Epoxidized esters)
Epoxidized soya oils (see Epoxidized esters)
1,2-Epoxybutane, 4-16
Ethyl chloride, 4-61
Ethylene dibromide (see 1,2-Dibromoethane)
Ethylene dichloride (see 1,2-Dichloroethane)
Ethylene oxide, 4-11
Ethylenimine (see Aziridine)

FD&C Yellow No. 5, 4-236
Formaldehyde, 4-84

1,4,5,6,7,7-Hexachloro-5-norbornene-2,3-dicarboxylic anyhdride (see Chlorendic anhydride)
Hydrazine, 4-171
Hydrazine hydrate, 4-171
Hydrazobenzene, 4-173
Hydrogen peroxide, 4-119
Hydroxylamine sulfate, 4-185

Isobutyraldehyde, 4-85

Ketene, 4-102

Lauroyl chloride, 4-110
Lauroyl peroxide, 4-122

Table 4-2
(continued)

Maleic anhydride, 4-103
Methyl chloride, 4-143
Methyl chloroform, 4-62
4,4'-Methylenebis(N,N-dimethylaniline), 4-207
Methylene chloride, 4-142
Methyl ethyl ketone peroxide, 4-122
(Mixed alkyl)phenoxypoly(ethyleneoxy)ethyl chloride, 4-156
Mixed linear alcohols, ethoxylated and phosphated, 4-45
Monochlorobenzene, 4-150
Monochloroparaffins (C_{10} - C_{14}), 4-63

N-Nitrosodiphenylamine, 4-197
Nonylphenol, ethoxylated and phosphated, 4-45

Octyl epoxytallates (see Epoxidized esters)

Perchloroethylene (see Tetrachloroethylene)
Peroxyacetic acid, 4-121
N-Phenyl-2-naphthylamine, 4-207
Phosgene, 4-99
Phthalic anhydride, 4-100
Propionaldehyde, 4-87
Propylene chlorohydrins, 4-73
Propylene dichloride (see 1,2-Dichloropropane)
Propylene oxide, 4-12

Salicylaldehyde, 4-90

Tetrabromophthalic anyhdride, 4-108
Tetrachloroethylene, 4-130
Tetrachlorophthalic anhydride, 4-108
Tetrafluoroethylene, 4-135
Tri-(2-butoxyethyl)phosphate, 4-47
Tributyl phosphate, 4-47
1,1,1-Trichloroethane (see Methyl chloroform)
Trichloroethylene, 4-132
Tri(2-chloroethyl)phosphate, 4-47
Tri(2-chloropropyl)phosphate, 4-47
Tricresyl phosphate, 4-47
Triethyl phosphate, 4-47
Trimellitic anhydride, 4-106
Trioctyl phosphate, 4-47
Triphenyl phosphate, 4-47
Tris(2,3-dibromopropyl)phosphate, 4-44
TRIS (see Tris(2,3-dibromopropyl)phosphate)

Vanillin, 4-90
Vinyl chloride, 4-129
Vinylidene chloride (see 1,1-Dichloroethylene)

1. Class I: Alkylating Agents

a. Class IA: Epoxides

The chemicals in this group are those with a known or estimated annual production of one million pounds or more. Because they have use patterns which apply for the most part to the chemical rather than to the group, most of the discussions are on individual chemicals.

Ethylene oxide

Ethylene oxide production amounted to 3893 million pounds in 1974 with sales of 457 million pounds (12%), and 4467 million pounds in 1975 with sales of 409 million pounds (9%). As the sales percentages show, most of the ethylene oxide is consumed captively by the producer to produce other chemicals. Imports in 1974 were 4 million pounds, mostly from Canada. Exports have been relatively small, peaking at 35 million pounds in 1972 (no data for 1974 or 1975 are available).

The U.S. 1974 consumption pattern for ethylene oxide was as follows: ethylene glycol, 59%; acyclic nonionic surface-active agents, 8%; glycol ethers, 7%; ethanolamines, 6%; diethylene glycol, 5%; cyclic nonionic surface-active agents, 5%; polyethylene glycol, 3%; triethylene glycol, 2%; polyether polyols, 2%; and others (choline and choline chloride, ethylene chlorohydrin, hydroxyethyl starch, arylethanolamines, acetal copolymer resins, and cationic surface-active agents), 3%. Consumption of ethylene oxide for these uses is expected to increase an average of 4.7-5.2% per year to 1980 In 1975, approximately 100 thousand pounds of ethylene oxide (less than .01% of total production) was used in its only non-intermediate use: as a fungicidal fumigant in the postharvest treatment of black walnut meats, copra, and whole spices, and in the treatment of books, scientific equipment and supplies (made of glass, metals, plastics, rubber, or textiles), drugs, leather, motor oil, paper, soil, straw, clothing, furs, furniture, and transportation equipment. This use is expected to grow at an average annual rate of 3.5-5% to 1980. Carbon disulfide and aluminum phosphide (which yields phosphine gas on exposure to moisture) have been used as commodity and space fungicidal fumigants and presumably could be used as substitutes for ethylene oxide, although carbon disulfide can pose a fire hazard in its use.

Propylene oxide

Production of propylene oxide in 1975 amounted to 1524 million pounds; 110 million pounds were exported, 21 million pounds were imported, and 16 million pounds were used from inventories, resulting in an approximate domestic consumption of 1450 million pounds. Approximately 60% of total production (914 million pounds) was used captively as a chemical intermediate; the remaining 40% was sold to others chiefly for the manufacture of specialty polyether polyols. The U.S. 1975 consumption pattern for propylene oxide was as follows: polyether polyols (for use in manufacture of polyurethane resins), 59%; propylene glycol, 21%; polyether polyols for the manufacture of surface-active agents, hydraulic brake fluids, lubricants for rubber molds and textile fibers, heat transfer fluids, metalworking fluids, and compression lubricants, 7%; dipropylene glycol, 3%; glycol ethers, 2%; synthetic glycerin, 1.8%; and others including isopropanolamines, propylene carbonate, hydroxypropyl cellulose, and hydroxypropyl starch, 6.2%. Small amounts of propylene oxide are used as a stabilizer for nitrocellulose lacquers, as a fumigant, and as a food preservative.

U.S. consumption of propylene oxide is expected to increase at an average growth rate of 9-10.5% from 1975 to 1980. Because so little propylene oxide is consumed in non-intermediate uses, no information was found on future growth rates or possible substitutes for propylene oxide in these applications.

Epichlorohydrin

The U.S. production of epichlorohydrin in 1973 has been estimated at 340 million pounds consisting of 160 million pounds (47%) of crude epichlorohydrin (which is captively used to manufacture synthetic glycerin) and 180 million pounds of refined epichlorohydrin. The U.S. 1973 consumption pattern for refined epichlorohydrin is as follows: manufacture of epoxy resins, 72%; epichlorohydrin elastomers, 3%; glycidyl ethers and modified epoxy resins, 3%; wet-strength resins, 3%; water treatment resins, 2.8%; surfactants, 2.2%; miscellaneous applications, 6%; and exports, 7%. Import statistics are not available for 1973. Imports for 1974 were 0.5 million pounds. The amount of epichlorohydrin used in epoxy resins is believed to be 54% captive, and the remaining uses, all of which are chemical intermediate uses, are based on purchased epichlorohydrin.

The consumption of crude epichlorohydrin for the production of synthetic glycerin is expected to continue to show essentially no growth in the future. The use of epichlorohydrin in epoxy resins is expected to increase 8-9% annually, in elastomers, 8-9% annually, and 4-5% annually in all other uses. The overall rate for crude and refined is expected to be 4-5%.

Alkyl glycidyl ethers

These compounds are manufactured by only one U.S. company so information on the total quantity produced is not available. However, an estimated

21-25 million pounds of alkyl (predominantly C_{12} and C_{14}) glycidyl ethers were consumed in the U.S. in 1975 for the captive production of alkyl glyceryl ether sulfonates. These sulfonates have unique detersive properties and are used as surfactant components in several types of products: shampoos, combination soap-syndet toilet bar soap, and light-duty liquid detergents. An unknown quantity (probably much smaller than the amount used for surfactant production) of these alkyl glycidyl ethers is used for other purposes. Recommended uses include use as reactive diluents for epoxy resin systems, as stabilizers for PVC resins, and as stabilizers for chlorinated paraffins and other halogenated products.

The annual growth rate for the use of these alkyl glycidyl ethers in the manufacture of the ether sulfonates is estimated at 8-9% to 1982. There are no known substitutes for the glycidyl ethers in this process; however, there presumably are other surfactants with properties similar to the end product, the ether sulfonates. No information was found on future growth rates or possible substitutes for the alkyl glycidyl ethers in the non-surfactant applications.

Epoxidized esters

This group of epoxidized compounds are used as plasticizers (primarily in PVC resins) and will be discussed together. The production of all epoxidized esters amounted to 154 million pounds in 1974, and dropped to 95 million pounds in 1975 due to the decreased production of PVC resins in 1975. The types of epoxidized esters included in 1974 were as follows (production in millions of pounds in parentheses): epoxidized soya oils (127); epoxidized linseed oil (5.5); octyl (n-octyl and 2-ethylhexyl) epoxytallates (14.9); and epoxidized tall oils, octyl epoxystearates, and other epoxidized esters (6.5).

These epoxidized esters are used as plasticizers in PVC formulations where they also function as heat and light stabilizers acting in synergism with barium-cadmium-zinc stabilizers. They are used as plasticizers in resin applications where resistance to leaching by soapy water and resistance to migration into adjoining materials is desired. Epoxidized soybean oils are FDA-approved for use in contact with food, and are thus used in some food-related PVC products. They are also used in PVC products for medical applications, and in adhesive-backed films (e.g., those used for tapes).

Future use of epoxidized esters is dependent on the markets for PVC products and the availability of the necessary refined grades of raw materials from fats and oils. The estimated annual growth rate for these plasticizers in the period from 1976 to 1980 is 7.6-10.8%.

These epoxidized esters serve a dual purpose in PVC resins: plasticization and stabilization to heat and light. As plasticizers, their permanence and resistance to leaching are important. The polymeric plasticizers, mostly adipic acid-based polyesters of very low residual functionality, also exhibit good resistance to migration and extraction. Heat stabilizers used in PVC include metal soaps (barium, cadmium, calcium, and zinc), organotin compounds (the dioctyl tin derivative has been sanctioned by the FDA for use in food packaging applications), lead compounds, nitrogen compounds (diphenyl thiourea and others), organophosphites, and phenols. Light stabilizers used in PVC resins are usually the monohydroxybenzophenones, the hydroxyphenylbenzotriazoles, and the substituted acrylates. Which, if any, of these plasticizers and stabilizers could be substituted for epoxidized esters in PVC depends on a number of factors including processability, the resin's intended use, other additives used in the resin, and cost.

1,2-Epoxybutane

The estimated production of 1,2-epoxybutane (butylene oxide) in 1974 was 10 million pounds. The principal use for this compound has been as a corrosion inhibitor (acid scavenger) in chlorinated solvents such as methyl chloroform and trichloroethylene at levels of 3-8%. Its use is expected to decline to approximately one million pounds in 1980. Other compounds used as inhibitors in these solvents include nitromethane, N-methylpyrrole, 1,4-dioxane, 1,3-dioxolane, sec-butanol, and other higher alcohols.

Endrin

Production data for this compound are not reported separately. It has been used exclusively as an insecticide and consumption for this purpose in 1974 has been estimated at 1.2 million pounds. Most of this consumption is believed to have been supplied by imports. The insecticide was used on cotton and other field crops. A notice of Rebuttable Presumption Against Registration (RPAR) and continued registration of pesticide products containing endrin was issued on July 27, 1976. The final decision on the RPAR is scheduled for May 1977. Numerous insecticides have been proposed as substitutes for endrin, with the choice of substitute depending on the specific application.

Other epoxy compounds

These compounds are of several chemical types: olefin oxides, including styrene oxide, vinyl cyclohexene dioxide, and 3,4-epoxycyclohexylmethyl 3,4-epoxycyclohexane carboxylate; glycidyl ethers, including allyl glycidyl ether, butyl glycidyl ether, and phenyl glycidyl ether; and esters, including glycidyl methacrylate. No information could be found for the production volume or growth rates for these compounds other than that their annual production is greater than one thousand pounds. They are used as reactive diluents in uncured epoxy resins to reduce the viscosity of the uncured system for ease in casting, adhesive, and laminating applications. Possible substitutes include non-reactive diluents such as solvents (e.g., xylene), dibutyl phthalate, monomeric styrene, and low-molecular-weight polystyrenes. In addition, phenols are used as reactive or non-reactive diluents depending on the intended method of cure.

EPOXIDES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
75218	Ethylene oxide	4467 x 10^6 lbs./1975/T75p	27 (delivered)	1206	I
75569	Propylene oxide	1524 x 10^6 lbs./1975/T75p	23 (f.o.b. plant)	351	I
106898	Epichlorohydrin	340 x 10^6 lbs./1973/SRI	42 (delivered)	143	I, II
8013078	Epoxidized soy oils	77 x 10^6 lbs./1975/T75p	48 (T75p)	37	--
--	Alkyl (predominantly C_{12} and C_{14}) glycidyl ethers	21-25 x 10^6 lbs./(1975/SRI (consumption)	--	--	--
--	Octyl epoxytallates	14.9 x 10^6 lbs./1974/T74	40 (T74)	6	--
106887	1,2-Epoxybutane	10 x 10^6 lbs./1974/SRI	--	--	--
8016113	Epoxidized linseed oils	5.5 x 10^6 lbs./1974/T74	--	--	--
72208	Endrin	1.2 x 10^6 lbs./1974/SRI (consumption)	300 (delivered)	3.6	I, II

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*Taken from Chemical Marketing Reporter, Feb. 4, 1977, reflecting the list prices prevailing for large lots. Values designated as coming from Synthetic Organic Chemicals, United States Production and Sales (T74 or T75p, p=preliminary), are unit sales value which is calculated from total quantities sold (the sum of the large quantities sold on a contractual basis and smaller quantities sold intermittently) and total sales value (the sum of the values of sales at contract prices and list prices).

Class: Alkylating Agents, Epoxides 2/17/77

EPOXIDES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Prod./Year/Source
--	Epoxidized tall oils	>1000 lbs./1974/T74
--	Polyacrylated linseed oil epoxide	>1000 lbs./1974/T74
81210	Dicyclopentadiene diepoxide	>1000 lbs./1976/SRI
96093	Styrene oxide	>1000 lbs./1974/T74
106843	Octyl epoxystearates	>1000 lbs./1974/T74
106876	Vinyl cyclohexene dioxide	>1000 lbs./1976/SRI
106901	Glycidyl acrylate	>1000 lbs./1974/T74
106912	Glycidyl methacrylate	>1000 lbs./1974/T74
106923	Allyl glycidyl ether	>1000 lbs./1974/T74
121391	Ethyl 3-phenylglycidate	>1000 lbs./1976/SRI
122601	Phenyl glycidyl ether	>1000 lbs./1974/T74
286204	Cyclohexene oxide	>1000 lbs./1976/SRI
556525	Glycidol	>1000 lbs./1974/T74
2186245	Cresyl glycidyl ether	>1000 lbs./1975/SRI
2386870	3,4-Epoxycyclohexylmethyl 3,4-epoxycyclohexane carboxylate	>1000 lbs./1976/SRI
2426075	1,2,7,8-Diepoxyoctane	>1000 lbs./1974/T74

EPOXIDES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Prod./Year/Source
2426086	Butyl glycidyl ether	>1000 lbs./1974/T74
3132647	Epibromohydrin	>1000 lbs./1976/SRI
3234284	1,2-Epoxytetradecane	>1000 lbs./1974/T74
7320378	1,2-Epoxyhexadecane	>1000 lbs./1974/T74
29804226	cis-7,8-Epoxy-2-methyloctadecane; Disparlure	>1000 lbs./1976/SRI

EPOXIDES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
--	1,2,6,7-Diepoxyheptane
--	4,5-Epoxy-3-hydroxyvaleric acid β-lactone
--	2,3-Epoxy-2-methylpropyl acrylate
--	Hexaepoxysqualene
60571	Dieldrin (production discontinued in 1975)
77838	α,β-Epoxy-β-methylhydrocinnamic acid, ethyl ester
96082	Limonene dioxide
101906	Diglycidyl resorcinol ether
106832	n-Butyl epoxystearate
106865	1-Vinyl-3,4-epoxycyclohexane
141377	3,4-Epoxy-6-methylcyclohexylmethyl 3,4-epoxy-6-methylcyclohexanecarboxylate
277065	1,2,3,4-Diepoxycyclohexane
286624	Epoxycyclooctane
286759	1,2,5,6-Diepoxycyclooctane
765344	Glycidaldehyde
930223	1,2-Epoxybutene-3
1464535	Diepoxybutane
1686142	α-Pinene oxide
1888897	1,2,5,6-Diepoxyhexane
1954285	Triethylene glycol diglycidyl ether
1984776	Dodecanoic acid, glycidyl ester
2443392	cis-9,10-Epoxystearic acid

Class: Alkylating Agents, Epoxides

EPOXIDES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name
2751099	Oleandomycin triacetate
2917988	1,4-Bis(2,3-epoxypropyl)piperazine
3012699	9,10,12,13-Diepoxystearic acid
3083258	(2,2,2-Trichloroethyl)oxirane
3130196	Bis(3,4-epoxy-6-methylcyclohexylmethyl)adipate
3234262	2,3-Epoxyoctane
3483394	Epoxyethylcyclohexane
3765284	2-(2-(3,3-Dimethyloxiranyl)ethenyl)-2,3-dimethyloxirane
3775857	Ethylene glycol bis(2,3-epoxy-2-methylpropyl)ether
3922905	Oleandomycin
4016119	Ethyl glycidyl ether
4051278	1,2,4,5-Diepoxypentane
5431334	Glycidyl oleate
5696173	1,1'-Bis(2,3-epoxypropyl)-4,4'-bipiperidine
5796509	Indan epoxide
7144652	(((1,1'-Biphenyl)-2-yloxy)methyl)oxirane
7163395	Cyclobuta(1",2":3,4;4",3":3',4')dicyclopenta(1,2-b:1',2'-b')bisoxirene, decahydro-
7460846	Glycidyl stearate
7487287	Bis(2,3-epoxy-2-methylpropyl)ether
10008603	Limonene monoxide
17526748	Hexanoic acid, glycidyl ester
23255698	Fusarenon-x

b. Class IB: Lactones

γ-Butyrolactone is the only chemical in this class with an estimated annual production greater than one million pounds. Production data for γ-butyrolactone are not published, but consumption is estimated to have been 31 million pounds in 1974. U.S. imports of γ-butyrolactone for 1974 were 75,000 lbs., mostly from the United Kingdom. U.S. export data for γ-butyrolactone are not published separately.

γ-Butyrolactone is used primarily as a chemical intermediate for vinylpyrrolidone, which is both homo- and co-polymerized to make polymers whose principal use is as film formers in hair sprays. These polymers are also used in the pharmaceutical industry as a tablet binder and coating agent and as a clarifying agent in the beer and wine industry. γ-Butyrolactone also is used as a chemical intermediate for N-methyl-2-pyrrolidone (an extraction solvent and polymer solvent) and for the herbicide 4-(2,4-dichlorophenoxy)butyric acid. γ-Butyrolactone is used as a solvent in many diverse applications, including as a polymer solvent (polyacrylonitrile, polyvinyl chloride, polyvinylcarbazole, polystyrene, polyamides, and cellulose acetate), in the textile industry as a spinning and coagulating solvent for polyacrylonitrile, as a solvent for many chemical reactions, and as a selective solvent (e.g., for acetylene) in the petroleum industry. No data are available as to the relative amounts of γ-butyrolactone consumed in these applications.

No specific data could be found on which to base an estimated growth rate for γ-butyrolactone consumption.

There are no known substitutes which could replace γ-butyrolactone in its chemical intermediate uses. However, substitutes do exist for the resulting products: (1) polyvinylpyrrolidone -- other film forming ingredients used in hair sprays include dewaxed shellac, carboxylated vinyl acetate resins, and acrylic copolymer resins; tablet binders in use include tragacanth, acacia, starch paste, and methylcellulose; tablet coatings can be formed by syrup and a film-forming agent such as gelatin, acacia, or methylcellulose; beer and wine have been clarified by the addition of bentonite; (2) 4-(2,4-dichlorophenoxy)butyric acid -- other herbicides such as Bolan® or dinoseb probably could be substituted.

Since a solvent is selected for its unique properties in any given process, it is beyond the scope of this discussion to investigate possible substitutes for γ-butyrolactone in each of its various solvent applications. Aqueous sodium thiocyanate and dimethylformamide have been used as spinning solvents for polyacrylonitrile. Most amorphous polymers are soluble in a number of different solvents depending on the hydrogen-bonding capacity of the solvent and on the solubility parameters of the polymer. These properties have been studied extensively by polymer technologists and a suitable substitute solvent for most polymers can be found in the polymer literature. Substitutes for γ-butyrolactone in its non-polymer-solvent applications could also be selected from solubility tables in the literature depending on the compound and process in question.

Class: Alkylating Agents: Lactones

LACTONES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
96480	γ-Butyrolactone	31×10^6 lbs./1974/SRI (consumption)	85 (works)	26	--

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*Taken from Chemical Marketing Reporter, April 11, 1977, reflecting the list prices prevailing for large lots.

Class: Alkylating Agents: Lactones

LACTONES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
104676	4-Hydroxyundecanoic acid, γ-lactone	29×10^3lbs./1975/T75
152750	D & C Red No. 21 (Eosine acid)	25×10^3lbs./1975/T75
91645	Coumarin	25×10^3lbs./1974/SRI (consumption)
119846	3,4-Dihydrocoumarin	23×10^3lbs./1975/T75
104610	4-Hydroxynonanoic acid, γ-lactone	7×10^3lbs./1975/SRI (consumption)
52017	Spironolactone	>1000 lbs./1977/SRI
71636	Digitoxin	>1000 lbs./1975/T75
71670	Sodium sulfobromophthalein	>1000 lbs./1977/SRI
77065	Gibberelic acid	>1000 lbs./1975/T75
77098	Phenolphthalein	>1000 lbs./1975/T75
87058	4-Methyl-7-ethoxycoumarin	>1000 lbs./1975/T75
90802	Glucono-δ-lactone	>1000 lbs./1975/T75
92477	6-Methylhydrocoumarin	>1000 lbs./1975/T75
92488	6-Methylcoumarin	>1000 lbs./1975/T75
104507	4-Hydroxyoctanoic acid, γ-lactone	>1000 lbs./1975/T75
105215	4-Hydroxyheptanoic acid, γ-lactone	>1000 lbs./1977/SRI
108292	γ-Valerolactone	>1000 lbs./1975/T75
115399	3',3",5',5"-Tetrabromophenolphthalein, ethyl ester	>1000 lbs./1975/T75
118081	Hydrastine	>1000 lbs./1977/SRI
128621	L-α-Narcotine (Noscapine)	>1000 lbs./1975/T75
502443	Caprolactone	>1000 lbs./1975/T75
518456	Fluorescein (D & C Yellow No. 7)	>1000 lbs./1975/T75

Class: Alkylating Agents: Lactones

LACTONES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
518478	Fluorescein sodium (C.I. Acid Yellow 73)	>1000 lbs./1975/T75
520456	Dehydroacetic acid	>1000 lbs./1977/SRI
674828	Diketene (Ketene dimer)	>1000 lbs./1975/T75
1076386	4-Hydroxycoumarin	>1000 lbs./1975/T75
4418262	Sodium dehydroacetate	>1000 lbs./1977/SRI

Class: Alkylating Agents: Lactones

LACTONES WITH ANNUAL PRODUCTION LESS THAN CNE THOUSAND POUNDS

CAS No.	Chemical Name
53394	Oxandrolone
54717	Pilocarpine hydrochloride
57578	β-Propiolactone
92137	Pilocarpine
92455	3-Chlorocoumarin
93356	β-Umbelliferone
148721	Pilocarpine nitrate
435972	Phenprocoumon
518401	4',5'-Diidofluorescein
630886	Fluorescein chloride
695067	γ-Hexalactone
705862	δ-Decalactone
706149	γ-Decalactone
713951	δ-Dodecalactone (Stage I dossier)
1111393	Acetyldigitoxin
2305057	γ-Dodecalactone
3902714	Trioxsalen
3068880	β-Butyrolactone
7774472	4,4-Dibutyl-γ-butyrolactone

c. Class IC: Aziridines

The parent compound of this group, aziridine (also called ethylenimine) is the only one with an annual production greater than one million pounds. Currently, there is only one U.S. manufacturer and its annual production is estimated to be three million pounds. It is believed that aziridine is no longer exported from the U.S. but small quantities may be imported from West Germany.

Approximately 50% of the aziridine produced in the U.S. is polymerized to polyethylenimine which contains less than 1 ppm residual monomer. Polyethylenimine has been used principally as a flocculant in water treatment, in the paper industry (where it is used as a wet-strength additive), as an adhesion promoter in adhesives, and in the textile industry (to improve dyeing and printing, for waterproofing, and to impart antistatic properties). Most of the remaining 50% of the aziridine produced is used as a chemical intermediate in drug, cosmetic, and dye manufacture, in the production of N-2-hydroxyethyl ethylenimine (a modifier of polymers for coatings, textiles, etc.), and as an intermediate and monomer for oil additive compounds, ion exchange resins, coating resins, adhesives, polymer stabilizers, and surfactants. No information was found on the amounts of aziridine used in the individual applications, or on trends in market growth.

All indications are that aziridine is used almost exclusively as a chemical intermediate to provide one or more aziridinyl- $(\overline{CH_2CH_2\text{-}N}\text{-})$ or ethyleneimino- $(\text{-}CH_2CH_2NH\text{-})$ substituents. The cationic nature of the products and the other properties imparted to the finished product (e.g., adhesion promotion, waterproofing) presumably could be accomplished using other chemicals but the cost of manufacture would probably be considerably higher.

Class: Alkylating Agents, Aziridines

AZIRIDINES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price, ¢/lb.	Market Value, Million $	Dossiers
151564	Aziridine (Ethylenimine)	3×10^6 lbs./1973/SRI	--	--	--

Class: Alkylating Agents, Aziridines

AZIRIDINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
1072522	N-2-Hydroxyethyl ethyleneimine (2-(1-Aziridinyl)ethanol)	>10x10^{4} lbs./1973/SRI (consumption)
57396	Tris(2-methyl-1-aziridinyl)phosphine oxide	>1000 lbs./1975/T75
57409	Bis(2-methyl-1-aziridinyl)phenylphosphine oxide	>1000 lbs./1977/SRI
75558	2-Methylaziridine (Propylenimine)	>1000 lbs./1975/T75 (Stage I dossier)
2549679	2-Ethyl ethyleneimine	>1000 lbs./1977/SRI
3527557	Hexa(2-methyl-1-aziridinyl)-1,3,5-phosphotriazine	>1000 lbs./1977/SRI
13009911	Tris(2-methyl-1-aziridinyl)-1,3,5-triazine	>1000 lbs./1977/SRI

Class: Alkylating Agents, Aziridines

AZIRIDINES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
51183	2,4,6-Tris(1-aziridinyl)-sym-triazine (Triethylenemelamine)
52244	Tris(1-aziridinyl)phosphine sulfide (Stage I and II dossiers)
52460	Hexa(1-aziridinyl)-1,3,5-phosphotriazine (Apholate)
68768	Tris(aziridinyl)-para-benzoquinone
545551	Tris(1-aziridinyl)phosphine oxide
800248	2,5-Bis(1-aziridinyl)-3,6-bis(2-methoxyethoxy)-para-benzoquinone
2168685	Bis(1-aziridinyl)morpholinophosphine sulfide

d. Class ID: Alkyl Sulfates

This class has been confined to the dialkyl esters, only two of which are of industrial importance, dimethyl sulfate and diethyl sulfate. Exact figures of production volume for these chemicals are not available. Prior to 1975, diethyl sulfate was a chemical intermediate in the production of ethyl alcohol from ethylene using sulfuric acid. This process is no longer used. Dimethyl sulfate and diethyl sulfate are presently used as alkylating agents to convert active-hydrogen compounds such as phenols, amines, and thiols to the corresponding alkyl derivatives. Except in the case of synthesizing quaternary ammonium salts by alkylating amines where it may be important that the quaternary be in the form of the methosulfate or ethosulfate salt, the corresponding alkyl halides can be used for these alkylations. Methyl chloride and ethyl chloride are the most likely substitutes.

Class: Alkylating Agents, Alkyl Sulfates

ALKYL SULFATES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
64675	Diethyl sulfate (Stage I, II dossiers)	>1000 lbs./1975/T75
77781	Dimethyl sulfate (Stage I, II dossiers)	>1000 lbs./1975/T75

Class: Alkylating Agents, Alkyl Sulfates

ALKYL SULFATES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
598050	Di-n-propyl sulfate
625229	Di-n-butyl sulfate
814404	Methyl ethyl sulfate
2973106	Di-isopropyl sulfate
5867958	Ethyl n-butyl sulfate
--	Bis(2-chloroethyl) sulfate
--	Bis(chloromethyl) sulfate
--	Didecyl sulfate
--	Ditetradecyl sulfate
--	Ethyl n-propyl sulfate
--	Methyl chloromethyl sulfate

e. Class IE: Sultones

This small group of chemicals does not have any members with annual U.S. production greater than one million pounds. The production of 1,3-propanesultone was estimated at 1000 pounds in 1973, but the only producer ceased production in 1975. The accompanying table summarizes the available data for this class.

Revised 5/77

Class: Alkylating Agents, Sultones

CAS No.	Chemical Name	Price, ¢/lb.	Annual Prod./Year/Source	Market Value, Million $	Dossiers
81083	o-Sulfobenzoic acid, cyclic anhydride	--	>1000 lbs./1975/T75	--	--
143748	Phenol,4,4-(3H-2,1-Benzoxathiol-3-ylidene)di-,S,S-dioxide (phenolsulfonphthalein)	--	>1000 lbs./1975/T75	--	--
1120714	1,2-Oxathiolane,2,2-dioxide (1,3-propanesultone)	--	prodn. discontinued in 1975	--	--
1633836	1,4-Butanesultone	--	<1000 lbs./1977/SRI	--	--

f. Class IF: Aryl Dialkyl Triazenes

This small class of compounds has no members with annual production greater than one million pounds. The three substituted phenylazo sarcosine derivatives which are produced in commercial quantities appear to be used solely as chemical intermediates. The two companies which produce these chemicals are both dye manufacturers but no evidence was found that they are used as dye intermediates.

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Class: Aklylating Agents, Aryl Dialkyl Triazenes

ARYL DIALKYL TRIAZENES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
103219	N-(p-Tolylazo)sarcosine	>1000 lbs./1977/SRI
120047	N-((5-Chloro-2-methoxyphenyl)azo)sarcosine	>1000 lbs./1977/SRI
136287	N-((5-Chloro-ortho-tolyl)azo)sarcosine	>1000 lbs./1977/SRI

Class: Alkylating Agents, Aryl Dialkyl Triazenes

ARYL DIALKYL TRIAZENES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
86180	N-(4-Benzamido-6-methoxy-meta-tolyl)-N-(methylazo)glycine
7203909	3,3-Dimethyl-1-(4-chlorophenyl)triazene
7203910	3,3-Dimethyl-1-(4-carboxyphenyl)triazene
7227910	3,3-Dimethyl-1-phenyltriazene
7227932	3,3-Dimethyl-1-(4-hydroxyphenyl)triazene
19992699	3,3-Dimethyl-1-(3-pyridyl)triazene
21600420	3,3-Dimethyl-1-(3-pyridyl-N-oxide)triazene
37599716	3,3-Dimethyl-1-(3-hydroxyphenyl)triazene
--	3,3-Dimethyl-1-(4-acetamidophenyl)triazene
--	3,3-Dimethyl-1-(4-bromophenyl)triazene
--	3,3-Dimethyl-1-(4-carbethoxyphenyl)triazene
--	3,3-Dimethyl-1-(4-fluorophenyl)triazene
--	3,3-Dimethyl-1-(4-methoxyphenyl)triazene
--	3,3-Dimethyl-1-(4-nitrophenyl)triazene
--	3,3-Dimethyl-1-(meta-tolyl)triazene
--	3,3-Dimethyl-1-(ortho-tolyl)triazene
--	3,3-Dimethyl-1-(2,4,6-tribromophenyl)triazene
--	3,3-Dimethyl-1-(2,4,6-trichlorophenyl)triazene

Class: Alkylating Agents, Aryl Dialkyl Triazenes

ARYL DIALKYL TRIAZENES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name
--	3,3-Diethyl-1-phenyltriazene
--	3,3-Diethyl-1-(3-pyridyl)triazene
--	3-Methyl-3-(2-hydroxyethyl)-1-phenyltriazene
--	3-Methyl-3-(2-sulfatoethyl)-phenyltriazene

g. Class IG: Diazoalkanes

This small class of compounds has no members with annual production greater than either one million or one thousand pounds. Diazomethane is a laboratory reagent used to methylate DNA in biological studies and to methylate a wide variety of organic compounds, but it is not sold as the compound itself, but in the form of three precursors, one of which, N-methyl-N-nitroso-p-toluenesulfonamide (CAS No. 80115), apparently has an annual production greater than one thousand pounds. Another precursor, N,N'-dimethyl-N,N'-dinitrosoterephthalamide (CAS No. 133551), has an annual production greater than one thousand pounds, but is mostly used as a blowing agent for rubbers and plastics. The third precursor, N-methyl-N'-nitro-N-nitrosoguanidine or MNNG (CAS No. 70257), is apparently produced in quantities less than one thousand pounds per year.

Class: Alkylating Agents, Diazoalkanes

CAS No.	Chemical Name	Annual Prod./Year/Source
334883	Diazomethane	<1000 lbs./1977/SRI
1117960	Diazoethane	<1000 lbs./1977/SRI
54043684	Diazoisobutane	<1000 lbs./1977/SRI
--	1-Diazodecane	<1000 lbs./1977/SRI
--	1-Diazohexane	<1000 lbs./1977/SRI
--	1-Diazopropane	<1000 lbs./1977/SRI

h. Class IH: Phosphoric Acid Esters

Of the 20 compounds in this class with an annual production (or consumption) greater than one million pounds, six--monocrotophos, dichlorvos, naled, phosphamidon, crotoxyphos, and crufomate--are used only as pesticides, and will not be discussed further. Of the remaining 14 compounds, tris(2,3-dibromopropyl)phosphate will be discussed individually; the two surface-active agents, nonylphenol, ethoxylated and phosphated, and mixed linear alcohols, ethoxylated and phosphated, will be discussed together; and the remaining eleven compounds, used chiefly as plasticizers, will be discussed together.

Tris(2,3-dibromopropyl)phosphate

In recent years, an estimated 10 million pounds of tris(2,3-dibromopropyl)phosphate (known as TRIS) have been produced annually in the U.S. Data for U.S. imports and exports for TRIS are not published separately.

TRIS has been used principally as an additive to impart flame retardance to synthetic fibers and fabrics such as polyester, acetate and triacetate, and acrylics. Approximately 65% of total production has been used in these textile applications. The polyester and acetate and triacetate fabrics containing TRIS have been largely used for children's sleepwear to impart flame retardance to meet the standards FF 3-71 and FF-5-74 promulgated under the Flammable Fabrics Act. The acrylic fibers have been used in carpeting.

As a result of concern about the mutagenic and carcinogenic properties of TRIS, the manufacturers of this sleepwear stopped using TRIS-treated fabrics in January 1977 and the Consumer Product Safety Commission banned the sale of TRIS-treated sleepwear in April 1977.

TRIS has also been used to impart flame retardancy to a variety of other synthetic polymers, including rigid and flexible polyurethane foams, cellulose nitrate surface coatings, polystyrene, polyvinyl chloride, phenolics, intumescent and non-intumescent paints, paper coatings, and rubber. Although the use of TRIS has not been banned in these applications, two major suppliers of TRIS were reported to be dropping production and a third was undecided whether it would continue to market the product. In view of the present turmoil over its use, the production of TRIS is expected to decrease rapidly.

There is no comparable substitute additive flame retardant at present which will adequately retard the flammability of polyester, acetate and triacetate, and acrylic fabrics. However, other methods are available for retarding the flammability of 100% polyester and of acrylics by incorporating a flame retardant comonomer such as 2,5-dibromoterephthalic acid in polyesters or a halogenated comonomer such as vinyl chloride or vinyl bromide in acrylics (which are then called modacrylics).

Surface-Active Agents

The U.S. production of nonylphenol, ethoxylated and phosphated, was 7.4 million pounds in 1973, 7.4 million pounds in 1974, and 4.2 million pounds in 1975. The U.S. production of mixed linear alcohols, ethoxylated and phosphated, was approximately 4 million pounds in both 1973 and 1975, and 4.9 million pounds in 1974. Data on U.S. imports and exports for these surface-active agents are not available.

These polyoxyethylene phosphate esters, as they are also known, are prepared by reacting mixed linear alcohols or nonylphenol with ethylene oxide, forming a polyoxyethylene derivative, which is then converted to phosphate esters (a mixture of mono- and diesters) by reaction with phosphorus trichloride, phosphorus pentoxide, phosphorus oxychloride, or polyphosphoric acid. These phosphate esters and their salts are anionic surface-active agents used in a variety of applications where their foaming, emulsifying, wetting, and detergent properties and solubility and compatibility are of importance.

The nonylphenol-derived products are used in a variety of applications: (1) as detergent concentrates (where they impart good hard-surface detergency, moderate foaming, and retardation of rusting and corrosion); (2) in wax and resin floor finishes; (3) in heavy-duty, all-purpose liquid formulations; (4) in industrial cleaners; (5) as drycleaning detergents; (6) as polymerization emulsifiers in the production of polyvinyl acetate and acrylic films (where they promote clarity, heat and light stability, stable neutral pH, and corrosion inhibition in the finished polymer); and (7) as emulsifiers for pesticides.

The linear alcohol-derived products are used in the textile industry as surfactants in the mercerizing of cotton, as lubricating, softening, and antistatic agents for wool and synthetic fibers, as emulsifiers for cosmetic oils and creams and clear hair grooming gels, in liquid alkaline detergent compositions, and in liquid drain cleaners. No information was available on the relative amounts of these polyoxyethylene phosphate esters used in the above applications so no estimate could be made of the rate of growth in their consumption.

The number of possible substitutes for these polyoxyethylene phosphate esters in these myriad applications is not known. It seems likely that substitutes can be found, but probably only with a compromise as to effectiveness, performance, and cost.

Plasticizers

The U.S. production of the remaining eleven phosphate esters, used chiefly as plasticizers, has been estimated as follows (millions of pounds): tricresyl phosphate, 56 (1974), 51 (1975); tri(2-chloroethyl)phosphate and tri(2-chloropropyl)phosphate, 15-20 (1974); cresyl diphenyl phosphate, 11.1 (1974), 7-8 (1975); triethyl phosphate, 7 (1974); trioctyl phosphate, 3 (1974); tributyl phosphate, 2 (1974). Production has not been estimated for the remaining four compounds--tri(2-butoxyethyl)phosphate, triphenyl phosphate, diphenyl octyl phosphate, and diphenyl isodecyl phosphate--but it is believed that production of each was greater than one million pounds in 1974. Data on U.S. exports of these compounds are not published separately. U.S. imports of tricresyl phosphate totaled 29.5 thousand pounds in 1974 and 150.3 thousand pounds in 1975; and of cresyl diphenyl phosphate, 75.0 thousand pounds in 1974, 72.2 thousand pounds in 1975. Data on U.S. imports of the remaining compounds are not published separately.

The aryl and alkyl aryl phosphates are used chiefly as plasticizers. The acyclic phosphates are used in a variety of non-plasticizer specialty uses.

Tricresyl phosphate, cresyl diphenyl phosphate, and diphenyl isodecyl phosphate are chiefly used as plasticizers for polyvinyl chloride (PVC) resins to impart flame retardance, usually in conjunction with other plasticizers. Trioctyl phosphate is also used as a polyvinyl chloride plasticizer, but it has no flame retarding properties. These plasticized PVC resins are used in many products and applications, including floor and wall coverings, home furnishings, consumer goods, packaging, wire and cable, automotive seating and trim, and agricultural film. Cresyl diphenyl phosphate has been used as a gasoline additive, but this use has all but disappeared since phosphorus can poison the precious metal catalysts in the converters. Diphenyl octyl phosphate has FDA approval for use in contact with food, and is used as a plasticizer in packaging film. Triphenyl phosphate is used as a plasticizer in cellulose acetate plastics and as a component of a polyphenylene oxide-based engineering plastic. Tricresyl phosphate, dibutyl phenyl phosphate, and, to a lesser extent, tributyl phosphate, are used in hydraulic fluids. Tricresyl phosphate imparts flame-resistant qualities to the hydraulic fluid and is used in locations where fire could be especially dangerous, such as in mines. Tributyl phosphate has also been used as an antifoaming agent in ore separation, but this use has declined in recent years. Tri(2-chloroethyl)phosphate and tri(2-chloropropyl)-phosphate are used as flame retardants in polyurethanes, acrylic fibers, and in other polymer systems. Triethyl phosphate is used as a plasticizer in cellulose acetate plastics, as a flame-retardant additive in unsaturated polyester resins, and as a chemical intermediate for the insecticide, tetraethyl pyrophosphate (TEPP). Tri(2-butoxyethyl)-phosphate is added as a leveling agent to styrene-butadiene emulsions (high-styrene types) used as floor polishes, and is used to a lesser extent as a plasticizer in elastomers. No data are available as to the relative amounts of these phosphate esters used in these applications.

Because of their flame-retarding properties, the consumption of phosphate ester plasticizers is expected to increase 8.1% per year from 1976 to 1981.

Other plasticizers used with polyvinyl chloride resins include the phthalates, epoxidized oils, aliphatic dicarboxylic esters, and polymeric plasticizers. However, none of these impart flame retardancy to the resin. Antimony oxide can be used to flame retard vinyl resins where its pigmenting properties are acceptable.

Other fire-resistant hydraulic fluids presently used include oil-in-water or water-in-oil emulsions, and water-glycol formulations.

Class: Alkylating Agents, Phosphoric Acid Esters

6/77

PHOSPHORIC ACID ESTERS WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value Million $	Dossiers
1330785	Tricresyl phosphate	51×10^6 lbs./1975/SRI	69 (delivered)	35	I
115968	Tri(2-chloroethyl)phosphate	$15\text{-}20 \times 10^6$ lbs./1974/SRI	--	--	I
6145739	Tri(2-chloropropyl)phosphate		--	--	--
126727	Tris(2,3-dibromopropyl)phosphate	10×10^6 lbs./1976/SRI	100 (est.)	10 (est.)	--
78319	Cresyl diphenyl phosphate	$7\text{-}8 \times 10^6$ lbs./1975/SRI	62(T75)	5	--
78400	Triethyl phosphate	7×10^6 lbs./1974/SRI	60 (delivered)	4	--
6923224	Monocrotophos (Azodrin®)	4.2×10^6 lbs./1974/SRI (consumption)	2200/gal. (5 lbs./gal.)	18	I,II
--	Nonylphenol, ethoxylated and phosphated	4.2×10^6 lbs./1975/T75	63 (T75)	2.6	--
--	Mixed linear alcohols, ethoxylated and phosphated	4×10^6 lbs./1975/T75	75 (T75)	3	--
1806548	Trioctyl phosphate	3×10^6 lbs./1974/SRI	--	--	--
62737	Dichlorvos (Vapona®)	2.7×10^6 lbs./1974/SRI (consumption)	1200/gal. (2 lbs./gal.)	16	I,II
300765	Naled (Dibrom®)	2.3×10^6 lbs./1974/SRI (consumption)	4000/gal. (8 lbs./gal.)	11.5	--
126738	Tributyl phosphate	2×10^6 lbs./1974/SRI	88 (works)	1.8	--

Class: Alkylating Agents, Phosphoric Acid Esters

PHOSPHORIC ACID ESTERS WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value Million $	Dossiers
13171216	Phosphamidon (Dimecron®)	$1.5x10^6$ lbs./1974/SRI (consumption)	4980/gal. (8 lbs./gal.)	9	IA
7700176	Crotoxyphos (Ciodrin®)	$1.3x10^6$ lbs./1974/SRI (consumption)	690	9	--
999865	Crufomate (Ruelene®)	$1x10^6$ lbs./1974/SRI (consumption)	2200/gal. (13.5% active ingredient)	--	--
78513	Tri(2-butoxyethyl)phosphate	$>1x10^6$ lbs./1974/SRI	--	--	--
115866	Triphenyl phosphate	$>1x10^6$ lbs./1974/SRI	74 (frt. eqlzd.)	0.7	--
115888	Diphenyl octyl phosphate	$>1x10^6$ lbs./1974/SRI	--	--	--
29761215	Diphenyl isodecyl phosphate	$>1x10^6$ lbs./1974/SRI	--	--	--

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*Taken from Chemical Marketing Reporter, April 25, 1977, reflecting the list prices prevailing for large lots. Values designated as coming from Synthetic Organic Chemicals, United States Production and Sales are unit sales value which is calculated from total quantities sold (the sum of the large quantities sold on a contractural basis and smaller quantities sold intermittently) and total sales value (the sum of the values of sales at contract prices and list prices). Prices of pesticides are list prices per gallon of formulated product. The amount of pesticide per gallon of formulation is included in parentheses. By dividing the price by the lbs./gal., an estimated price/lb. of pesticide can be obtained. This estimate was used in calculating the market value. In the case of Crufomate, no estimate was possible because neither the lbs./gal. nor the weight of a gallon for formulated product were available.

Class: Alkylating Agents, Phosphoric Acid Esters

PHOSPHORIC ACID ESTERS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
7786347	Mevinphos (Phosdrin®)	$8\text{x}10^5$ lbs./1974/SRI (consumption)
2528361	Dibutyl phenyl phosphate	$7.3\text{x}10^5$ lbs./1975/T75 (sales)
--	Tridecyl alcohol, ethoxylated and phosphated	$6.7\text{x}10^5$ lbs./1975/T75
141662	Dicrotophos (Bidrin®)	$5\text{x}10^5$ lbs./1974/SRI (consumption)
141651	Phosphoric acid, bis(2-ethylhexyl)ester, sodium salt	$1.4\text{x}10^5$ lbs./1975/T75
107493	Tetraethyl pyrophosphate	$1\text{x}10^5$ lbs./1974/SRI (consumption)
961115	Stirophos (Rabon®)	$1\text{x}10^5$ lbs./1974/SRI (consumption)
58979	5'-Uridylic acid	>1000 lbs./1977/SRI
63376	5'-Cytidilic acid	>1000 lbs./1977/SRI
78433	Tris(2,3-dichloropropyl)phosphate	>1000 lbs./1977/SRI
130405	Riboflavine 5'-phosphate, sodium salt	>1000 lbs./1975/T75
298077	Phosphoric acid, bis(2-ethylhexyl)ester (2-Ethyl-1-hexanol, hydrogen phosphate)	>1000 lbs./1975/T75
522407	Diethylstilbestrol diphosphate	>1000 lbs./1975/T75
812000	Methyl dihydrogen phosphate	>1000 lbs./1975/T75

Class: Alkylating Agents, Phosphoric Acid Esters

PHOSPHORIC ACID ESTERS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
819830	Sodium glycerophosphate (Stage I dossier)	>1000 lbs./1977/SRI
838857	Phenyl hydrogen phosphate	>1000 lbs./1975/T75
1070037	Phosphoric acid, mono(2-ethylhexyl)ester	>1000 lbs./1977/SRI
1319693	Potassium glycerophosphate (Stage I dossier)	>1000 lbs./1977/SRI
1336001	Calcium glycerophosphate (Stage I dossier)	>1000 lbs./1977/SRI
3900047	Hexyl phosphate	>1000 lbs./1975/T75
5116949	Tridecyl phosphate	>1000 lbs./1975/T75
5412259	Bis(2,3-dibromopropyl)phosphate	>1000 lbs./1977/SRI
7057923	Didodecyl hydrogen phosphate	>1000 lbs./1975/T75
13270650	5-Phosphorylribose 1-pryophosphate	>1000 lbs./1977/SRI
--	2,2-Bis(chloromethyl)trimethylene bis(di(2-chloroethyl)phosphate)	>1000 lbs./1975/T75
--	Butyl alcohol, ethoxylated and phosphated	>1000 lbs./1977/SRI
--	Butyl ethyl phosphate	>1000 lbs./1975/T75
--	n-Butyl hydrogen phosphate	>1000 lbs./1975/T75

Class: Alkylating Agents, Phosphoric Acid Esters

PHOSPHORIC ACID ESTERS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
--	Butyl phosphate, potassium salt	>1000 lbs./1975/T75
--	Decyl alcohol, ethoxylated and phosphated	>1000 lbs./1975/T75
--	Decyl, dodecyl, and octyl phosphate, morpholine salt	>1000 lbs./1975/T75
--	Diethylene glycol bis(di-2-chloroethyl)phosphate	>1000 lbs./1975/T75
--	Dinonylphenol, ethoxylated and phosphated	>1000 lbs./1975/T75
--	Dinonylphenol, ethoxylated and phosphated, potassium salt	>1000 lbs./1975/T75
--	Dodecyl alcohol, ethoxylated and phosphated	>1000 lbs./1975/T75
--	Dodecylphenol, ethoxylated and phosphated	>1000 lbs./1975/T75
--	2-Ethylhexanol, ethoxylated and phosphated	>1000 lbs./1975/T75
--	2-Ethylhexyl polyphosphate	>1000 lbs./1975/T75
--	2-Ethylhexyl polyphosphate, sodium salt	>1000 lbs./1975/T75
--	Glycerol monoester of mixed fatty acids, phosphated	>1000 lbs./1975/T75
--	Hexylphenol, ethoxylated and phosphated	>1000 lbs./1975/T75
--	Hexyl phosphate, potassium salt	>1000 lbs./1975/T75

Class: Alkylating Agents, Phosphoric Acid Esters

PHOSPHORIC ACID ESTERS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
--	Hexyl polyphosphate, potassium salt	>1000 lbs./1975/T75
--	Iso-octyl hydrogen phosphate	>1000 lbs./1975/T75
--	Isopentyl alcohol, ethoxylated and phosphated	>1000 lbs./1977/SRI
--	Mixed alkyl phosphates	>1000 lbs./1975/T75
--	Mixed alkyl phosphates, diethanolamine salt	>1000 lbs./1975/T75
--	Monooleyl phosphate	>1000 lbs./1975/T75
--	Nonylphenol, ethoxylated and phosphated, barium salt	>1000 lbs./1975/T75
--	9-Octadecenyl alcohol, ethoxylated and phosphated	>1000 lbs./1975/T75
--	Octadecyl alcohol, ethoxylated and phosphated	>1000 lbs./1975/T75
--	Octylphenol, ethoxylated and phosphated	>1000 lbs./1975/T75
--	Octyl phosphate, alkylamine salt	>1000 lbs./1975/T75
--	Octyl phosphate, ethoxylated	>1000 lbs./1975/T75
--	Octyl polyphosphate	>1000 lbs./1975/T75
--	Octyl polyphosphate, potassium salt	>1000 lbs./1975/T75
--	Oleyl hydrogen phosphate	>1000 lbs./1975/T75

Class: Alkylating Agents, Phosphoric Acid Esters

PHOSPHORIC ACID ESTERS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
--	Phenol, ethoxylated and phosphated	>1000 lbs./1975/T75
--	Polyalkylene glycol, phosphated	>1000 lbs./1975/T75
--	Polyhydric alcohol, ethoxylated and phosphated	>1000 lbs./1975/T75
--	Polypropylene glycol, phosphated	>1000 lbs./1975/T75

Class: Alkylating Agents, Phosphoric Acid Esters

PHOSPHORIC ACID ESTERS WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
57034	Glycerophosphoric acid
115899	Methyl diphenyl phosphate
131997	5'-Inosinic acid
312936	Pregna-1,4-diene-3,20-dione,9-fluoro-11,17-dihydroxy-16-methyl-21-(phosphonooxy)-, (11.beta, 16.alpha)-
360634	Pregna-1,4-diene-3,20-dione, 9-fluoro-11,17-dihydroxy-16-methyl-21-(phosphonooxy)-, (11.beta, 16.beta)-
512561	Phosphoric acid, trimethyl ester (Trimethyl phosphate)
3991739	Mono-n-octyl phosphate
5324129	Mono(2,3-dibromopropyl)phosphate
7546283	Propanoic acid, 2-(phosphonoxy)-, calcium salt
7558625	1,2,3-Propanetriol, 1-(dihydrogen phosphate), manganese salt (Manganese glycerophosphate)
19045795	Mono-n-octyl phosphate, dipotassium salt
--	Bis(2,3-dibromopropyl)allyl phosphate
--	Decyl polyphosphate, sodium salt

Class: Alkylating Agents, Phosphoric Acid Esters

PHOSPHORIC ACID ESTERS WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name
--	Diallyl 2,3-dibromopropyl phosphate
--	Diethyl vinyl phosphate
--	2-Ethylhexyl phosphate, triethanolamine salt
--	Iso-octyl phosphate
--	Octylphenol, ethoxylated and phosphated, magnesium salt
--	Tri(castor oil alkyl)phosphate

i. Class II: Halogenated Saturated Hydrocarbons

This class includes compounds with two or more carbon atoms since Halogenated Methanes are discussed in subclass IVB.

There are nine members of this class with an annual U.S. production greater than one million pounds. However, one of these, 1,2-dibromo-3-chloropropane, is used almost exclusively as a pesticide and will not be discussed further.

Two of the chemicals are fluorocarbons which have been reviewed in great depth in two reports prepared in 1975: "Economic Significance of Fluorocarbons," Office of Business Research and Analysis, Bureau of Domestic Commerce, U.S. Department of Commerce (December 1975) and "Preliminary Economic Impact Assessment of Possible Regulatory Action to Control Atmospheric Emissions of Selected Hydrocarbons" (PB 247115). These two reports cover so many facets of the subject that SRI felt that it would be inappropriate to try to prepare a condensed version for this report. The information regarding uses of the fully halogenated fluorocarbons was recently brought up to date as part of the notice of proposed rulemaking which the EPA published in the Federal Register on May 13, 1977 (pp. 24542-24549). In view of the availability of these documents, it was felt that the time and funds which would be required to prepare a market forecast on the fluorocarbons would be better spent on other parts of this research request.

Because the other six chemicals have different use patterns, they will be discussed individually.

1,2-Dichloroethane

U.S. production of this chemical which is more commonly known as ethylene dichloride) in recent years has been as follows (billions of pounds): 1974 (9.17); 1975 (7.98); and 1976 (7.92). U.S. imports of

1,2-dichloroethane in 1974 are estimated to have been 75 million pounds and U.S. exports totaled 369 million pounds in 1974 and 130 million pounds in 1975.

The estimated U.S. domestic consumption pattern for 1,2-dichloroethane in 1976 was: 86% as an intermediate for vinyl chloride; approximately 3% each as an intermediate for 1,1,1-trichloroethane and ethyleneamines; 2% each as an intermediate for tetrachloroethylene, 1,1-dichloroethene, and trichloroethylene, and as a lead scavenger for motor fuels.

In late 1975, future growth in total U.S. consumption of 1,2-dichloroethane, and in consumption for synthesis of vinyl chloride were both estimated at 4% annually through 1979. Since over 90% of the vinyl chloride produced in the U.S. is made via 1,2-dichloroethane, the information on future growth presented under Vinyl Chloride applies to the 1,2-dichloroethane used for this production also. Any growth in the use of 1,2-dichloroethane to make 1,1,1-trichloroethane because of the expected increased use of this chemical in metal cleaning would largely be offset by decreases in the amount needed to produce the two competitive metal cleaning solvents, tetrachloroethylene and trichloroethylene. The consumption of 1,2-dichloroethane as a motor fuel lead scavenger is likely to decrease if proposed reductions of the average lead content of gasoline are implemented.

Less than 10% of U.S. production of vinyl chloride is based on the addition of hydrogen chloride to acetylene, a process used for 48% of U.S. production in 1963. This process could be used to replace the route via 1,2-dichloroethane. Other processes based on chlorination of either ethylene and recycled chloroethanes or of ethane are used commercially in other countries.

Ethyl chloride

U.S. production of ethyl chloride in recent years has been as follows (millions of pounds): 1974 (662); 1975 (575); and 1976 (642). U.S. imports of ethyl chloride amounted to only 4917 pounds in 1975. Data on exports are not available but exports are believed to be larger than imports.

More than 80% of total 1973 U.S. production of ethyl chloride was used for the production of the gasoline antiknock agent, tetraethyl lead. The remainder was used for a variety of miscellaneous applications, probably including: (1) manufacture of ethyl cellulose plastics, dyes, and pharmaceuticals; (2) use as a solvent; and (3) use as a refrigerant.

The future level of production of ethyl chloride will largely be dependent on the consumption of tetraethyl lead as a gasoline antiknock agent. U.S. domestic consumption of lead alkyls (mostly tetraethyl lead) decreased from 660 million pounds (100% lead alkyls basis) in 1973 to 548 million pounds in 1975. If the EPA's program to reduce the lead content of gasoline to 0.5 gram per gallon by late 1979 is implemented, even larger decreases in the consumption of lead alkyls would result. Widespread adoption of an alternate antiknock agent, methylcyclopentadienyl manganese tricarbonyl, could make further inroads into the market for lead alkyls. However, development of catalyst systems for autos which are more tolerant of lead could have a counteracting effect.

Combined U.S. production of ethyl cellulose and the closely related ethyl hydroxyethyl cellulose (both of which are made with ethyl chloride) amounted to an estimated 13 million pounds in 1973. Domestic consumption totaled 10 million pounds, with 7 million pounds consumed in surface coatings and the remainder in plastics, adhesives, and inks. Other thermoplastic polymers could probably provide the light weight, toughness, and temperature stability required in the major markets for these ethyl cellulose plastics but the choice would depend on the particular use and the cost-effectiveness of the polymer.

Methyl chloroform

U.S. production of this chemical (which is also known as 1,1,1-trichloroethane) in recent years has been as follows (millions of pounds): 1974 (592); 1975 (459); and 1976 (575). In 1974, U.S. imports are believed to have been negligible and exports are estimated to have totaled 70 million pounds.

The estimated U.S. domestic consumption pattern for methyl chloroform in 1974 was: 71% as a cleaning solvent (for metals and other materials); 23% as an intermediate for production of 1,1-dichloroethylene; and 6% for miscellaneous uses (e.g., aerosol component, coolant in metal cutting oils, and carrier for lubricants).

Originally introduced for cold cleaning of various industrial products or machinery, methyl chloroform was adopted for use in vapor degreasing when a satisfactory inhibitor system was developed and growth in consumption in this area has increased rapidly. In 1974, only slightly more was being used for cold cleaning than for vapor degreasing. In late 1975, overall U.S. consumption of methyl chloroform was expected to increase at an average annual rate of 4% with use as a cleaning solvent providing essentially all of this growth (no growth in use as an intermediate for 1,1-dichloroethylene was expected) and use as a vapor degreasing solvent growing more rapidly than use in cold cleaning. In the light of the developments discussed under

Tetrachloroethylene and Trichloroethylene, it seems likely that these estimates will be exceeded and that methyl chloroform will become the major metal cleaning solvent but will not completely displace the others.

Monochloroparaffins (C_{10}-C_{14})

In the principal method used in the U.S. to manufacture the linear alkyl-benzene used for the production of the surface-active linear alkylate sulfonates, paraffins in the C_{10}-C_{14} range are treated with chlorine to produce a mixture of C_{10}-C_{14} monochloroparaffins which are mostly secondary alkyl chlorides with the formula $CH_3(CH_2)_xCHCl(CH_2)_yCH_3$ where $x + y = 7$ to 11. U.S. production of these monochloroparaffins in 1976 is estimated to have been greater than 280 million pounds. Since they are used exclusively to alkylate benzene to produce linear alkyl benzenes at the site of their production, there are no U.S. imports or exports.

The level of future production of the monochloroparaffins will depend on demand for the linear alkylbenzenes. Normal paraffin consumption for production of linear alkylbenzenes is expected to grow at an average annual rate of 2% through 1980 but whether the monochloroparaffin route will retain its present share of the total linear alkylbenzene plant capacity is not known. The alternative process, used in the largest single U.S. linear alkylbenzenes plant, starts with normal paraffins also, but dehydrogenates these to a mixture of olefins which is used to alkylate the benzene.

1,2-Dibromoethane

U.S. production of this chemical (which is more commonly known as ethylene dibromide) was 332 million pounds in 1974 and 275 million pounds in 1975. Data on U.S. imports and exports are not available but 1973 exports are estimated to have been about 100 million pounds.

By far the major use of 1,2-dibromoethane is as a lead scavenger in antiknock motor mixes. It is used in the mixes for automotive gasolines and competes with 1,2-dichloroethane in the mixes used in aviation gasoline. 1,2-Dibromoethane has a variety of small uses also: an estimated 5 million pounds were used as a fumigant (mostly on agricultural crops) in 1975; it is an intermediate in the production of vinyl bromide, a reactive fire retardant which has found some use in modacrylic fibers; small amounts are used as a solvent and for other chemical intermediate purposes.

In late 1976, one source estimated that U.S. consumption of 1,2-dibromoethane would drop at an average annual rate of 10% through 1980 as a result of a continued drop in the usage of lead-based antiknock motor mixes. As discussed under Ethyl chloride, the future prospects for such mixes do not look good.

The continued use of 1,2-dibromoethane as a fumigant is also in doubt since the EPA has included it in a list of pesticides which are candidates for an RPAR action. A notice of such action is required by October 1, 1977. If the action is taken, the final outcome could be limitations or banning of the use of 1,2-dibromoethane as a pesticide.

1,2-Dichloropropane

U.S. production of this chemical (also known as propylene dichloride) was 145.1 million pounds in 1974 and 84.2 million pounds in 1975. Combined U.S. imports of the 1,2-dichloro derivatives of ethane, propane, and butane amounted to 90.1 million pounds in 1974 (1,2-dichloroethane is estimated to have accounted for 75 million pounds of this) and 88 million pounds in 1975. Separate data on U.S. exports of 1,2-dichloropropane are not available.

No data on the U.S. consumption pattern for 1,2-dichloropropane are available. It is believed that the major use is as a chemical intermediate for the production of tetrachloroethylene and carbon tetrachloride. 1,2-Dichloropropane is also an ingredient of the proprietary fumigant D-D® (which contains 55-60% 1,3-dichloropropene plus lesser quantities of 1,2-dichloropropane, 2,3-dichloropropene, 3,3-dichloropropene, and related C_3 chlorinated hydrocarbons). U.S. consumption of this fumigant on agricultural crops is estimated to have been 35 million pounds in 1975.

The future level of U.S. production of 1,2-dichloropropane will depend on the future use of the chlorohydrin process for producing propylene oxide, which yields 1,2-dichloropropane as a byproduct. As discussed under Propylene chlorohydrins, the quantity of propylene oxide made by this route may increase somewhat even though the alternate route, catalytic peroxidation of propylene, is preferred for new installations. Whether the 1,2-dichloropropane produced as a byproduct will continue to be used primarily to produce tetrachloroethylene and carbon tetrachloride is problematical in view of the adverse developments discussed under Tetrachloroethylene and Carbon tetrachloride. The fumigant D-D® has met EPA requirements for re-registration but the use of 1,3-dichloropropene alone is expected to increase dramatically in the future at the expense of the D-D® mixture.

Revised 8/77

Class: Alkylating Agents, Halogenated Saturated Hydrocarbons

HALOGENATED SATURATED HYDROCARBONS WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
107062	1,2-Dichloroethane (Ethylene dichloride)	7977×10^6 lbs./1975/T75	8 (T75)	638	IA
75003	Ethyl chloride (Chloroethane)	575×10^6 lbs./1975/T75	10 (T75)	57.5	--
71556	Methyl chloroform (1,1,1-trichloroethane)	459×10^6 lbs./1975/T75	17 (T75)	78	I, II
--	Monochloroparaffins (C_{10}-C_{14})	$>280 \times 10^6$ lbs./1976/SRI	--†	--†	--
106934	1,2-Dibromoethane (Ethylene dibromide)	275×10^6 lbs./1975/T75	27 (T75)	74.3	I,II,IA
78875	1,2-Dichloropropane	84.2×10^6 lbs./1975/T75	4 (T75)	3.37	--
26523648	Trichlorotrifluoroethane	64×10^6 lbs./1974/BDC‡	--	--	--
96128	1,2-Dibromo-3-chloropropane	25×10^6 lbs./1975/SRI	--	--	I, II
76142	1,2-Dichlorotetrafluoroethane	23×10^6 lbs./1974/BDC‡	--	--	--

*Taken from Chemical Marketing Reporter, April 25, 1977, reflecting the list prices prevailing for large lots. Values designated as coming from Synthetic Organic Chemicals, United States Production and Sales (T75), are unit sales value which is calculated from total quantities sold (the sum of the large quantities sold on a contractual basis and smaller quantities sold intermittently) and total sales value (the sum of the values of sales at contract prices and list prices).

†The monochloroparaffins are not offered for sale.

‡Economic Significance of Fluorocarbons, December 1975, Bureau of Domestic Commerce Staff Study, Office of Business Research and Analysis, Bureau of Domestic Commerce, U.S. Department of Commerce.

Class: Alkylating Agents, Halogenated Saturated Hydrocarbons

HALOGENATED SATURATED HYDROCARBONS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
58899	Lindane (1,2,3,4,5,6-hexachlorocyclohexane)	600×10^3 lbs./1974/SRI (consumption)
67721	Hexachloroethane	>1000 lbs./1976/SRI
74964	Ethyl bromide (Bromoethane)	>1000 lbs./1975/T75
75036	Ethyl iodide (Iodoethane)	>1000 lbs./1975/T75
75263	2-Bromopropane	>1000 lbs./1975/T75
75296	2-Chloropropane	>1000 lbs./1976/SRI
75343	1,1-Dichloroethane	>1000 lbs./1976/SRI
75376	1,1-Difluoroethane	>1000 lbs./1975/T75
75683	1-Chloro-1,1-difluoroethane	>1000 lbs./1975/T75
76153	Chloropentafluoroethane	>1000 lbs./1975/T75
78762	2-Bromobutane	>1000 lbs./1975/T75
78773	1-Bromo-2-methylpropane	>1000 lbs./1977/SRI
78864	2-Chlorobutane	>1000 lbs./1976/SRI
79005	1,1,2-Trichloroethane	>1000 lbs./1975/T75

Class: Alkylating Agents, Halogenated Saturated Hydrocarbons

HALOGENATED SATURATED HYDROCARBONS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
79276	1,1,2,2-Tetrabromoethane	>1000 lbs./1975/T75
79345	1,1,2,2-Tetrachloroethane	>1000 lbs./1976/SRI
96184	1,2,3-Trichloropropane	>1000 lbs./1975/T75
106945	1-Bromopropane	>1000 lbs./1975/T75
107813	2-Bromopentane	>1000 lbs./1975/T75
107824	1-Bromo-3-methylbutane	>1000 lbs./1976/SRI
108850	Cyclohexyl bromide	>1000 lbs./1977/SRI
109659	1-Bromobutane	>1000 lbs./1975/T75
109693	1-Chlorobutane	>1000 lbs./1975/T75
109648	1,3-Dibromopropane	>1000 lbs./1976/SRI
109706	1-Bromo-3-chloropropane	>1000 lbs./1975/T75
110521	1,4-Dibromobutane	>1000 lbs./1975/T75
110532	1-Bromopentane	>1000 lbs./1976/SRI
111240	1,5-Dibromopentane	>1000 lbs./1976/SRI
111251	n-Hexyl bromide	>1000 lbs./1977/SRI
111831	n-Octyl bromide	>1000 lbs./1977/SRI

Class: Alkylating Agents, Halogenated Saturated Hydrocarbons

HALOGENATED SATURATED HYDROCARBONS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
111859	1-Chlorooctane	>1000 lbs./1976/SRI
112298	n-Decyl bromide	>1000 lbs./1977/SRI
112823	1-Bromohexadecane	>1000 lbs./1977/SRI
112890	n-Octadecyl bromide	>1000 lbs./1977/SRI
124732	1,2-Dibromotetrafluoroethane	>1000 lbs./1975/T75
143157	n-Dodecyl bromide	>1000 lbs./1977/SRI
151677	2-Bromo-2-chloro-1,1,1-trifluoroethane (Halothane)	>1000 lbs./1975/T75
507200	2-Chloro-2-methylpropane	>1000 lbs./1976/SRI
540545	1-Chloropropane	>1000 lbs./1976/SRI
542187	Cyclohexyl chloride	>1000 lbs./1975/T75
626879	1,4-Dibromopentane	>1000 lbs./1975/T75
629049	n-Heptyl bromide	>1000 lbs./1977/SRI
693583	n-Nonyl bromide	>1000 lbs./1977/SRI
930289	Cyclopentyl chloride	>1000 lbs./1976/SRI
3386332	n-Octadecyl chloride	>1000 lbs./1977/SRI
4333566	Cyclopropyl bromide	>1000 lbs./1976/SRI
25497294	Chlorodifluoroethane	>1000 lbs./1976/SRI

Class: Alkylating Agents, Halogenated Saturated Hydrocarbons

HALOGENATED SATURATED HYDROCARBONS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
--	Chlorotrifluoroethane	>1000 lbs./1976/SRI
--	Dichlorohexafluoropropane	>1000 lbs./1976/SRI
--	Dichlorotrifluoroethane	>1000 lbs./1975/T75
--	Hexabromocyclododecane	>1000 lbs./1977/SRI
--	1-Iodoperfluorohexane	>1000 lbs./1975/T75
--	Pentabromo-6-chlorocyclohexane	>1000 lbs./1975/T75
--	n-Tetradecyl bromide	>1000 lbs./1977/SRI
--	n-Undecyl bromide	>1000 lbs./1977/SRI

Class: Alkylating Agents, Halogenated Saturated Hydrocarbons

HALOGENATED SATURATED HYDROCARBONS WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
75810	1,2-Dibromo-1,1-dichloroethane
76119	Difluorotetrachloroethane
76120	1,1,2,2-Tetrachloro-1,2-difluoroethane
76164	Hexafluoroethane
78751	1,2-Dibromopropane
107846	1-Chloro-3-methylbutane
115253	Octafluorocyclobutane
--	1-Bromoadamantane
--	2-Bromo-2-methylpropane
--	Chloroheptafluoropropane
--	Cyclopentyl bromide
--	n-Decyl chloride
--	Dibromodifluoroethane

Class: Alkylating Agents, Halogenated Saturated Hydrocarbons

HALOGENATED SATURATED HYDROCARBONS WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name
--	n-Dodecyl chloride
--	n-Hexyl chloride
--	n-Hexyl iodide
--	Isopropyl iodide
--	Pentachloroethane
--	n-Tetradecyl chloride
--	1,1,1-Trichloropropane

j. Class IJ: Halogenated Alkanols

There are only two members of this class with an annual U.S. production greater than one million pounds. Because these chemicals have different use patterns, they will be discussed individually.

Propylene chlorohydrins

U.S. production of this mixture of 1-chloro-2-propanol and 2-chloro-1-propanol produced by the chlorohydrination of propylene is estimated to have been greater than 1.78 billion pounds in 1976. It is believed that there are no U.S. imports or exports of propylene chlorohydrins.

Approximately 60% of the propylene oxide produced in the U.S. is made by the reaction of propylene with hypochlorous acid, followed by treatment of the resulting propylene chlorohydrins with slaked lime or caustic soda. The other 40% is made by the catalytic peroxidation of propylene. The peroxidation process makes more efficient use of propylene and does not produce undesirable waste streams (e.g., weak calcium chloride solutions). Consequently, it is the process of choice for new installations.

Propylene chlorohydrins apparently have no commercially significant uses other than as an intermediate for propylene oxide. U.S. consumption of propylene oxide is expected to grow at an annual average rate of 9-10% through 1980, largely as a result of growth in propylene oxide-derived polyols used in polyurethanes and propylene glycols used in polyester resins.

The quantity of propylene oxide produced by the chlorohydrination route may increase somewhat, even though its percentage of the total production does not increase, because the industry was operating at only about 65% of nameplate capacity as recently as 1975.

2,3-Dibromo-1-propanol

U.S. production of 2,3-dibromo-1-propanol is estimated to have been greater than 10 million pounds in 1976. Data on U.S. imports and exports are not available.

Until recent years, it is believed that practically all 2,3-dibromo-1-propanol was used as an intermediate for the manufacture of the flame retardant, tris(2,3-dibromopropyl)phosphate (so-called TRIS). More recently it is believed to have found some use as an intermediate for reactive flame retardants (e.g., dibromopropyl acrylate and methacrylate) and as a reactive flame retardant itself.

Although TRIS has found some use as a flame retardant in a variety of other applications, it is believed that its major application since 1973 has been in the treatment of fabrics for use in infants' and children's sleepwear. As a result of concern about the mutagenic and carcinogenic properties of TRIS, the manufacturers of this sleepwear stopped using TRIS-treated fabrics in January 1977 and the Consumer Product Safety Commission banned the sale of TRIS-treated sleepwear in April 1977. Since that time, users of TRIS for other flame retarding purposes have announced decisions to stop using it. Consequently, it seems very likely that total U.S. production of 2,3-dibromo-1-propanol has already decreased dramatically and will continue to do so. Its use in reactive flame retardants for such products as polyurethane foams, which is believed to be still in the development stage, is likely to be adversely affected by the fact that 2,3-dibromo-1-propanol itself has been found to be mutagenic also.

Class: Alkylating Agents, Halogenated Alkanols

HALOGENATED ALKANOLS WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price, ¢/lb.	Market Value, Million $	Dossiers
127004	1-Chloro-2-propanol	>1783.8x10^6 lbs./1976/SRI*	--	--	--
78897	2-Chloro-1-propanol				
96139	2,3-Dibromo-1-propanol	>10x10^6 lbs./1976/SRI	--	--	--

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*Production estimate is for the mixed propylene chlorohydrins produced as intermediates in the chlorohydrin route to propylene oxide.

Revised 7/77

Class: Alkylating Agents, Halogenated Alkanols

HALOGENATED ALKANOLS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
57158	1,1,1-Trichloro-2-methyl-2-propanol	>1000 lbs./1975/T75
75898	2,2,2-Trifluoroethanol	>1000 lbs./1977/SRI
96231	1,3-Dichloro-2-propanol	>1000 lbs./1977/SRI
96242	3-Chloro-1,2-propanediol	>1000 lbs./1975/T75
107073	2-Chloroethanol (Ethylene chlorohydrin)	>1000 lbs./1975/T75
115208	2,2,2-Trichloro-1-ethanol	>1000 lbs./1977/SRI
540512	2-Bromoethanol	>1000 lbs./1977/SRI
920661	Hexafluoro-2-propanol	>1000 lbs./1977/SRI
3296900	2,2-Bis(bromomethyl)-1,3-propanediol	>1000 lbs./1975/T75

Class: Alkylating Agents, Halogenated Alkanols

HALOGENATED ALKANOLS WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
75809	2,2,2-Tribromoethanol
371620	2-Fluoroethanol
453134	1,3-Difluoro-2-propanol
554109	3-Iodo-1,2-propanediol
598185	2-Bromo-1-propanol
616239	2,3-Dichloro-1-propanol
624470	2-Iodoethanol
4704772	3-Bromo-1,2-propanediol
19686738	1-Bromo-2-propanol
--	Tribromoneopentyl glycol

k. Class IK: Halogenated Ethers

There are only two members of this class with an annual U.S. production greater than one million pounds: bis(2-chloro-1-methylethyl)ether and bis(2-chloroethoxy)methane. Because these chemicals have different use patterns, they will be discussed individually.

Bis(2-chloro-1-methylethyl)ether

The 1975 U.S. production of bis(2-chloro-1-methylethyl)ether is estimated to have been greater than 30 million pounds. This chemical, which is also known as dichloroisopropyl ether and bis(2-chloroisopropyl)ether, is one of several by-products formed in the so-called chlorohydrin method used commercially to convert propylene to propylene oxide. In the chlorohydrin method, propylene and hypochlorous acid are reacted to give propylene chlorohydrin and this is treated with calcium hydroxide to produce propylene oxide. Prior to 1969, essentially all propylene oxide was made by the chlorohydrin process. At that time, another process, the peroxidation of propylene, was introduced which does not produce bis(2-chloro-1-methylethyl) ether as a by-product. This process has been increasing in popularity and the percentage of announced propylene oxide nameplate capacity based on it is expected to reach 44% in mid-1977.

Data on U.S. imports and exports of bis(2-chloro-1-methylethyl)ether are not available.

In spite of the large quantity of byproduct bis(2-chloro-1-methylethyl) ether produced annually, it is believed that much of this chemical never is marketed. One of the major producers of propylene oxide via the chlorohydrin route reportedly collects and burns most of the byproduct bis(2-chloro-1-methylethyl)ether.

Bis(2-chloro-1-methylethyl)ether has found use primarily as a solvent (e.g., for fats, waxes, and greases; as an extractant; in paint and varnish removers; in spotting and cleaning solutions; and in textile processing). Its use as a chemical intermediate appears to have been very limited.

The quantity of bis(2-chloro-1-methylethyl)ether produced as a byproduct is not expected to change dramatically in the future. The proportion of this production which will be burned will presumably depend on whether other more profitable uses can be found for the chemical.

Bis(2-chloroethoxy)methane

The 1973 production of bis(2-chloroethoxy)methane is estimated to have been greater than 20 million pounds. This chemical, which is also known as dichloroethylformal, is believed to be produced by the reaction of formaldehyde with ethylene chlorohydrin and converted directly to polysulfide elastomers by reaction with sodium sulfide. It is not known to have any other uses and is not marketed in commercial quantities by any of the manufacturers of these polysulfide elastomers.

Data on U.S. imports and exports of bis(2-chloroethoxy)methane are not available.

Polysulfide elastomers fall into two categories: castable types and specialized solid types. Although bis(2-chloroethoxy)methane is believed to be one of the major intermediates for polysulfide elastomers, it is not known whether it is used to make both types of elastomers. The castable type elastomers, with an estimated U.S. consumption of 8.8 million pounds in 1976, are used primarily for sealants and caulks and also for flexible products and in rocket fuel binders. The specialized solid types, with an estimated U.S. consumption of 1.1 million pounds in 1976, are used for a variety of non-tire industrial uses where their excellent environmental resistance is required.

U.S. consumption of castable polysulfide elastomers has reportedly decreased dramatically in the last few years although consumption of all castable elastomers (mostly polyurethanes) has increased considerably. If this trend continues, production of bis(2-chloroethoxy)methane could decrease further. Competition for the sealants and caulks market comes mainly from polyurethane and silicone elastomers.

U.S. consumption of specialized solid polysulfide resins has reportedly held steady in recent years. Neoprene elastomers appear to be the major competition in markets requiring good environmental resistance properties.

Class: Alkylating Agents, Halogenated Ethers

HALOGENATED ETHERS WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price, ¢/lb.	Market Value, Million $	Dossiers
108601	Bis(2-chloro-1-methylethyl) ether (Dichloroisopropylether)	>30x10^6 lbs./1975/SRI	--	--	--
111911	Bis(2-chloroethoxy)methane (Dichloroethylformal)	>20x10^6 lbs./1973/SRI	--	--	--

Class: Alkylating Agents, Halogenated Ethers

HALOGENATED ETHERS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
76380	2,2-Dichloro-1,1-difluoroethyl methyl ether	>1000 lbs./1975/T75
107302	Chloromethyl methyl ether	>1000 lbs./1975/T75
110758	2-Chloroethyl vinyl ether	>1000 lbs./1975/T75
111444	Bis(2-chloroethyl) ether	>1000 lbs./1976/SRI
112265	1,2-Bis(2-chloroethoxy)ethane (Triglycol dichloride)	>1000 lbs./1974/T74
2032351	2-Bromo-1,1-diethoxyethane (Diethylbromoacetal; Bromoacetaldehyde diethyl acetal)	>1000 lbs./1976/SRI
4885023	Dichloromethyl methyl ether	>1000 lbs./1976/SRI

Class: Alkylating Agents, Halogenated Ethers

HALOGENATED ETHERS WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
97972	Chloroacetaldehyde dimethyl acetal
127902	Octachlorodi-n-propyl ether
542881	Bis(chloromethyl) ether
621625	Chloroacetaldehyde diethyl acetal
627429	2-Chloroethyl methyl ether
638562	1,1'-Oxybis(2-(2-chloroethoxy)ethane)
3188134	Chloromethyl ethyl ether
7252837	2-Bromo-1,1-dimethoxyethane (Dimethylbromoacetal; Bromoacetaldehyde dimethyl acetal)
13483186	1,2-Bis(chloromethoxy)ethane
38571732	1,2,3-Tris(chloromethoxy)propane
--	Perfluoropropyl vinyl ether

1. Class IL: Aldehydes

The chemicals in this group are those with a known or estimated annual U.S. production level of one million pounds or more. They are divided into two groups, industrial chemicals and flavor and fragrance chemicals.

Industrial Chemicals

This subset includes the following seven chemicals: formaldehyde, acetaldehyde, n-butyraldehyde and isobutyraldehyde, propionaldehyde, acrolein, and chloral. Because they have use patterns which apply for the most part to the chemical rather than to the subset, most of the discussions are on individual chemicals.

Formaldehyde

In 1976, U.S. production of formaldehyde, 37% by weight solution (all the following figures assume this concentration), amounted to 5,621 million pounds. In 1973, a U.S. production high of 6,424 million pounds was reported. Much of the U.S. formaldehyde production is captively consumed. In 1975, about 65% of total production was used internally by producing companies. U.S. imports of formaldehyde are negligible and amounted to only 50,000 pounds in 1976, and U.S. exports amounted to 35 million pounds.

U.S. consumption of formaldehyde amounted to about 5,586 million pounds in 1976 and is expected to grow at the rate of 4-5% per year during the next five years. The U.S. consumption pattern for formaldehyde is as follows: urea resins, 25.4%; phenolic resins, 24.3%; butanediol, 7.7%; acetal resins, 7.0%; pentaerythritol, 6.0%; hexamethylenetetramine, 4.5%; melamine resins, 4.2%; urea-formaldehyde concentrates, 3.6%; chelating agents, 3.6%; methylenedianiline and methylenediphenyl isocyanate, 2.6%; textile treating applications, 1.8%; pyridine chemicals, 1.3%; trimethylolpropane, 1.3%; nitroparaffin derivatives, 0.4%; and other miscellaneous applications, 6.3%.

U.S. consumption of formaldehyde in the manufacture of urea-formaldehyde resins is expected to remain static or decline by as much as 3% during 1976-1981. The phenol-formaldehyde resins market is expected to increase as a market for formaldehyde at 4-5% per year to become the largest end market by 1981.

Acetaldehyde

U.S. production of acetaldehyde was estimated as 1,100 million pounds in 1976. A production high of 1,652 million pounds was last reported in 1969. U.S. imports of acetaldehyde amounted to only nine thousand pounds in 1975. Exports data are not available; however, exports are believed to be negligible.

Acetaldehyde is used in the U.S. as a chemical intermediate for the production of acetic acid and derivatives (60%) and for other chemicals (40%) including: pyridine, peracetic acid, pentaerythritol, crotonaldehyde, chloral, 1,3-butylene glycol, lactic acid, and metaldehyde. U.S. production of acetaldehyde is expected to grow at an average annual rate of 2% per year during 1977-1980. Acetic acid and derivatives can also be produced by methanol carbonylation, which currently appears to be the preferred process. Increasing usage of this process could have an adverse affect on U.S. acetaldehyde consumption in the future.

n-Butyraldehyde and Isobutyraldehyde

In 1974, U.S. production of n-butyraldehyde and isobutyraldehyde amounted to 564.9 and 381.9 million pounds, respectively, In 1975, U.S.

production of n-butyraldehyde was reported as 533 million pounds. U.S. imports of butyraldehyde (isomer unspecified) amounted to 1.256 million pounds in 1975. U.S. exports data are not available.

n-Butyraldehyde and isobutyraldehyde are produced from propylene via the oxo process. Since n-butyraldehyde is the preferred isomer, process conditions are regulated to favor that isomer. It is generally believed that butyraldehyde production figures are significantly understated because most butyraldehyde is not isolated from the process en route to derivatives. Since isobutyraldehyde may be produced in larger quantities than desired, it may be burned as fuel or recycled by cracking it to propylene, carbon monoxide and hydrogen.

The U.S. consumption pattern for butyraldehydes (including both isomers) based on production statistics of derivatives is estimated to have been as follows in 1975: n-butyl alcohol, 40%; 2-ethylhexyl alcohol, 38%; isobutyl alcohol, 16%; and others, 6%. U.S. demand for butyraldehydes is expected to increase at an average annual rate of 5% per year during 1976-1980.

n-Butyraldehyde is used as a chemical intermediate to produce n-butyl alcohol (used primarily as a solvent in surface coatings), 2-ethylhexyl alcohol (used mainly as an intermediate for polyvinyl chloride plasticizers), and miscellaneous chemicals (including n-butyric acid and anhydride and polyvinyl butyral). n-Butyl alcohol can also be produced from the fermentation of molasses or other agricultural products.

Isobutyraldehyde is used as a chemical intermediate to produce isobutyl alcohol (used to make isobutyl acetate and plasticizers), as a solvent for protective coatings, and as a diluent-reactant in the manufacture of amino resins. Isobutyraldehyde is also used to produce neopentyl glycol and trimethylpentanol.

Propionaldehyde

Although production figures for propionaldehyde are not reported in the U.S., U.S. demand for propionaldehyde in 1975 is estimated to have been 310 million pounds per year. U.S. imports and exports data for propionaldehyde are not available.

The U.S. consumption pattern for propionaldehyde has been estimated as follows: propanol, 40%; propionic acid, 37%; other uses (including butyl acrylate, cellosolve, and other solvents), 23%.

Propionic acid is the end-use market with the highest potential for growth. Propionic acid is used in the U.S. as an animal feed grain preservative (30%) and for the manufacture of food preservatives (propionates), herbicides, and plastics (70%). Since only 2% of the corn feed crop is preserved with propionic acid (the rest is dried by burning propane), increased demand for propionic acid could result in large increases in propionaldehyde production. Other uses of propionic acid are expected to grow at an average annual rate of 7-8% in the next few years.

Acrolein

U.S. acrolein production in 1974 is estimated to have been 61 million pounds. However, the acrolein produced and consumed captively for the production of acrylic acid and esters is believed to have amounted to 100-150 million pounds. U.S. imports and exports data are not available.

Excluding the portion of unisolated acrolein, the U.S. consumption pattern for acrolein in 1974 was estimated as follows: glycerin, 50%; synthetic methionine, 25%; other applications, 25%.

U.S. consumption of acrolein for the manufacture of glycerin has remained essentially static since 1968 and is not expected to increase significantly. Glycerin is also produced by methods not using acrolein.

Acrolein demand for the manufacture of the two poultry feed additives, dl-methionine and methionine hydroxy analogue, calcium salt, was expected to double in 1976 as the result of the start-up of a new dl-methionine plant. Over half of the U.S. consumption of synthetic methionine is currently supplied by imports. U.S. demand for synthetic methionine is expected to grow at an annual average rate of 2-3% during the next several years. Methionine is also available from natural feedstuffs such as fishmeal.

Acrolein is also used for the manufacture of 1,2,6-hexanetriol and glutaraldehyde. Other miscellaneous applications for acrolein include its use in: the manufacture of glyceraldehyde, perfume, colloidal forms of metals, and numerous other organic compounds; as an aquatic herbicide, molluscicide, slimicide, and algicide; and in the etherification of food starch. Acrolein consumption for these applications is expected to increase at a rate of about 5% per year. Total production of isolated acrolein is expected to increase at a rate of 7-8% per year until 1979.

The major portion of acrolein produced in the U.S. is consumed captively in the production of acrylic acid and esters. It has been estimated that by 1977, about 77% of total U.S. acrylic acid and esters production operating capacity will be derived from captive acrolein. Acrylic acid and esters can also be manufactured from acetylene via the Reppe process.

Chloral

U.S. production figures for chloral are not available. U.S. consumption of chloral, based on data for the production of its derivatives, is estimated to have been over 30 million pounds in 1975. No U.S. imports of chloral are reported, although imports of chloral hydrate amounted to 105 thousand pounds in 1975. U.S. exports data for chloral are not available; however they are believed to be very small and sporadic.

The 1975 consumption pattern for chloral in the U.S. has been estimated as follows: DDT, 78%; other insecticides, 17%; pharmaceuticals, 4%; and herbicide, 1%.

Since 1972, when the EPA banned the use of DDT in the U.S. except for emergency use under Section 18 of FEPCA, most DDT production is exported. DDT exports amounted to 47.2 million pounds in 1975. During the period 1972-1975, U.S. DDT production levels are believed to have remained at annual levels of 50 million pounds. It is believed that these levels will remain static in the future.

Other insecticides manufactured from chloral include methoxychlor, DDVP, and naled. U.S. production of methoxychlor, which was estimated at 6-8 million pounds in 1973, is expected to increase at an average annual rate of 6% per year during the next several years. Because DDVP is an RPAR candidate, its future outlook is uncertain and its production will probably decrease.

Chloral is also consumed in the production of pharmaceuticals, primarily chloral hydrate. Small quantities of chloral are used to manufacture the herbicide, trichloroacetic acid.

Flavor and Fragrance Chemicals

This subset includes the following four chemicals which are used in the flavor and fragrance industries: salicylaldehyde, vanillin, cinnamaldehyde, and anisic aldehyde. Although information on the future outlook for each specific chemical is not available, total sales in the U.S.

flavor and fragrance industry are expected to increase at an average annual rate of 10% per year during the next five to seven years. About one-half of this growth rate could represent price increases only.

Salicylaldehyde

U.S. production of salicylaldehyde amounted to 4.6 million pounds in 1975, down from a 1974 production level of 5.25 million pounds. U.S. imports and exports data for salicylaldehyde are not available.

Salicylaldehyde is used as a chemical intermediate for the manufacture of coumarin, a fragrance used in perfumery. Salicylaldehyde has also been used to fortify violet perfumes. N,N'-Disalicylidene -1,2-propanediamine, a condensation product of salicylaldehyde and propylenediamine is used as metal deactivator in gasoline. Other reported uses for salicylaldehyde include: as a stabilizer for certain polymer compositions; as a fungicide and larvicide; in analytical chemistry; and as a flavoring agent in food.

Information on the outlook for U.S. salicylaldehyde production or for possible chemical substitutes is not available.

Vanillin

U.S. production of vanillin is currently estimated at 3.0-3.5 million pounds annually. U.S. imports of vanillin amounted to 2.9 million pounds in 1975. U.S. exports data for vanillin are not available. The current U.S. consumption pattern for vanillin is estimated as: flavoring agent, 50%; pharmaceutical intermediate, 50%.

Vanillin is used as a synthetic substitute for vanilla in flavoring foods such as syrups, chocolate, chewing gum, baked goods, candy, toppings, gelatins and puddings, ice cream, non-alcoholic beverages, and margarine. Vanillin is used as a chemical intermediate for the manufacture of pharmaceuticals, including l-dopa, steroids, and antidepressant drugs. Small amounts of vanillin are also used in electroplating.

Currently, one of the two U.S. vanillin manufacturers is closing down production due to problems with pollutants at its plant and that of the company supplying the raw material lignin used to manufacture vanillin. However, the other U.S. manufacturer will increase production of vanillin so that the market for vanillin will not change appreciably.

Increases in the price of vanilla beans may induce users to switch to vanillin, increasing vanillin demand. Information on possible chemical substitutes for vanillin is not available.

Cinnamaldehyde

U.S. production of cinnamaldehyde amounted to 1.75 million pounds in 1973. U.S. imports of cinnamaldehyde through principal U.S. customs districts amounted to 51.64 thousand pounds in 1974. Data for U.S. exports of cinnamaldehyde are not available.

Cinnamaldehyde is used as a flavoring agent in foods and as a chemical intermediate for the fragrance ingredient, cinnamaldehyde dimethyl acetal. Cinnamaldehyde is used as a cinnamon flavor in chewing gum, candy, baked goods, meats, condiments, non-alcoholic beverages, ice cream, liqueurs and cordials, and medicine. Its dimethyl acetal derivative is used in fragrances for soap (0.01%) (usual concentration of cinnamaldehyde dimethyl acetal in final product), detergent (0.002%), creams and lotions (0.003%), and perfume (0.08%). Cinnamaldehyde has also been used as a denaturant for ethanol.

Information on the outlook for U.S. cinnamaldehyde production or for possible chemical substitutes is not available.

Anisic aldehyde

U.S. production of anisic aldehyde in 1975 amounted to 1.103 million pounds with sales amounting to 1.065 million pounds. U.S. imports of anisic aldehyde through principal U.S. customs districts amounted to 1,455 pounds in 1975, down from 4,365 pounds in 1974. Data for U.S. exports of anisic aldehyde are not available.

Anisic aldehyde is used as a flavoring agent in foods and as an ingredient in fragrances. Anisic aldehyde is used in such flavor compositions as anise, caramel, chocolate, strawberry, and vanilla, for use in chewing gum, gelatins and puddings, baked goods, candy, non-alcoholic beverages, and ice cream. About 50 thousand pounds of anisic aldehyde are used annually in fragrances. It is used in the following products (the usual concentration in the final product is shown in parentheses): soap (0.03%); detergents (0.005%); creams and lotions (0.02%); and perfume (0.4%).

Information on the outlook for U.S. anisic aldehyde production or for possible chemical substitutes is not available.

Class: Alkylating Agents, Aldehydes

Revised 7/77

ALDEHYDES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
50000	Formaldehyde	4558×10^6 lbs. (37%)/1975/T75	5.35	244	I
75070	Acetaldehyde	1100×10^6 lbs./1976/SRI	18 (99%)	198	I
123728	n-Butyraldehyde	533×10^6 lbs./1975/T75	24	128	--
78842	Isobutyraldehyde	382×10^6 lbs./1974/T74	22.5	86	--
123386	Propionaldehyde	166×10^6 lbs./1973/SRI	25	42	--
107028	Acrolein	61×10^6 lbs./1974/SRI	31	19	I
75876	Chloral	31×10^6 lbs./1975/SRI (consumption)	36 (94% min.)	11	--
90028	Salicylaldehyde	4.6×10^6 lbs./1975/T75	250	11.5	--
121335	Vanillin	3×10^6 lbs./1976/SRI (est.)	475	14.3	I
104552	Cinnamaldehyde	1.8×10^6 lbs./1973/SRI	150	2.7	I, II
123115	Anisic aldehyde	1.1×10^6 lbs./1974/T74	345	3.8	--

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*Taken from Chemical Marketing Reporter, April 11, 1977, reflecting the list prices prevailing for large lots, f.o.b. New York.

Class: Alkylating Agents, Aldehydes

ALDEHYDES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Prod./Year/Source
106230	Citronellal	6.3×10^5 lbs./1975/T75
100527	Benzaldehyde	5.0×10^5 lbs./1972/SRI
1331926	Amyl cinnamic aldehyde	4.6×10^5 lbs./1975/T75
121324	Ethyl vanillin (Stage I dossier)	4.5×10^5 lbs./1972/SRI
107755	Hydroxycitronellal	3.3×10^5 lbs./1975/T75
141275	Citral	8.7×10^4 lbs./1973/T73
100107	p-(Dimethylamino)benzaldehyde	1.5×10^4 lbs./1975/T75
124130	Octanal	7×10^3 lbs./1975/T75
21866706	α-Methylcinnamaldehyde	4×10^3 lbs./1975/T75 (consumption)
66842	Glucosamine hydrochloride	>1000 lbs./1976/SRI
75901	Trifluoroacetaldehyde	>1000 lbs./1976/SRI
79027	Dichloroacetaldehyde	>1000 lbs./1976/SRI
89985	o-Chlorobenzaldehyde	>1000 lbs./1975/T75
93538	2-Phenylpropionaldehyde	>1000 lbs./1976/SRI
96173	2-Methylbutyraldehyde	>1000 lbs./1975/T75
97961	2-Ethylbutyraldehyde	>1000 lbs./1975/T75
103957	Cyclamen aldehyde	>1000 lbs./1975/T75
104096	p-Tolyl acetaldehyde	>1000 lbs./1975/T75
104530	3-Phenylpropionaldehyde	>1000 lbs./1976/SRI
104881	p-Chlorobenzaldehyde	>1000 lbs./1975/T75
106729	2,6-Dimethyl-5-heptenal	>1000 lbs./1975/T75
107891	3-Hydroxybutyraldehyde	>1000 lbs./1976/SRI

Class: Alkylating Agents, Aldehydes

ALDEHYDES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Prod./Year/Source
110418	Methylnonylacetaldehyde	>1000 lbs./1975/T75
110623	Valeraldehyde	>1000 lbs./1975/T75
111308	Glutaraldehyde (Stage I dossier)	>1000 lbs./1975/T75
112312	Capraldehyde	>1000 lbs./1975/T75
112447	Undecanal	>1000 lbs./1975/T75
112458	Undecylenic aldehyde	>1000 lbs./1976/SRI
112549	Lauraldehyde	>1000 lbs./1975/T75
120149	Veratraldehyde	>1000 lbs./1975/T75
122032	Cuminic aldehyde	>1000 lbs./1975/T75
122781	Phenyl acetaldehyde	>1000 lbs./1975/T75
123057	2-Ethylhexanal	>1000 lbs./1975/T75
123159	2-Methylvaleraldehyde	>1000 lbs./1975/T75
123739	Crotonaldehyde	>1000 lbs./1975/T75
124196	Nonanal	>1000 lbs./1975/T75
124254	Myristaldehyde	>1000 lbs./1975/T75
143146	9-Undecenal	>1000 lbs./1975/T75
505577	2-Hexenal	>1000 lbs./1975/T75
533675	D-2-Deoxyribose	>1000 lbs./1976/SRI
590863	Isopentaldehyde, mixed isomers	>1000 lbs./1975/T75
1335100	Hydrocinnamaldehyde	>1000 lbs./1976/SRI
1401690	Tylosin	>1000 lbs./1975/T75
4395920	p-Isopropylphenylacetaldehyde	>1000 lbs./1975/SRI

Class: Alkylating Agents, Aldehydes

ALDEHYDES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Prod./Year/Source
7492673	Citronelloxyacetaldehyde	>1000 lbs./1975/T75
9002817	Paraformaldehyde	>1000 lbs./1975/T75
10031820	p-Ethoxybenzaldehyde	>1000 lbs./1975/T75

Class: Alkylating Agents, Aldehydes

ALDEHYDES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
78988	Pyruvaldehyde
99729	2-(p-Tolyl)propionaldehyde
107200	Chloroacetaldehyde (Stage I dossier)
111717	Heptanal
120709	Phenoxyacetaldehyde
135024	o-Methoxybenzaldehyde
138556	Saffron
496037	2-Ethyl-3-hydroxyhexanal
590863	Isovaleraldehyde
881865	Vanillin acetate
947911	Diphenylacetaldehyde
2439443	3-Methyl-2-phenylbutyraldehyde
3913711	2-Decenal
4826624	2-Dodecenal
7774825	2-Tridecenal
7775000	3-(p-Isopropylphenyl)propionaldehyde
7779079	2,6-Dimethyloctanal
7786290	2-Methyloctanal
26254922	α-Ethylisovalderaldehyde

2. Class II: Acylating Agents

Eleven members of this class have annual U.S. production greater than one million pounds. Because these chemicals have different use patterns, they will be discussed individually, with the exception of tetrachloro- and tetrabromophthalic anhydride, which will be discussed together.

Acetic anhydride

U.S. production of acetic anhydride was 1.63 billion pounds in 1974 and 1.46 billion pounds in 1975. U.S. imports were 23 million pounds in 1974 and 20 million pounds in 1975. U.S. exports are believed to be negligible.

Acetic anhydride is used as a chemical intermediate in the manufacture of cellulose acetate and triacetate, aspirin, and other chemicals (including other cellulose esters). The manufacture of cellulose acetate and triacetate accounted for 90% of total acetic anhydride consumption (1490 million pounds). This cellullose acetate and triacetate was used to make textiles for apparel and home furnishings (approximately 60%) and for cigarette filters (approximately 40%). Approximately 1.4% of total acetic anhydride consumption (23 million pounds) was used to manufacture aspirin, and the remaining 8.6% (142 million pounds) was consumed in the manufacture of other chemicals, including other cellulose esters such as cellulose acetate butyrate and cellulose acetate propionate (resins used for surface coatings) and some specialty ester plasticizers such as acetyl ricinoleates. Future growth of acetic anhydride consumption is expected to be less than 1% per year to 1979.

There are no substitutes for acetic anhydride in the above-mentioned intermediate uses. However, the final products, i.e., cellulose acetate and triacetate, aspirin, cellulose acetate butyrate/propionate surface coatings, and specialty plasticizers could presumably all be replaced by other fabrics, antipyretics, or surface coatings, albeit with some loss in performance, comfort, or effectiveness.

Phosgene

U.S. production of phosgene was reported to be 728 million pounds in 1973, 867 million pounds in 1974, and 796 million pounds in 1975. It is believed that reported production has been 10-30% below actual production. Data on U.S. imports and exports of phosgene are not available.

Phosgene is an extremely poisonous and reactive gas, so it is usually produced and consumed captively at the point of production. It is used exclusively as a chemical intermediate in the manufacture of toluene diisocyanate, polymethylene polyphenylisocyanate, polycarbonate resins, and other chemicals. The consumption of phosgene for these intermediate uses has been estimated to have been 1066 million pounds in 1973 with 62% (658 million pounds) consumed for toluene diisocyanate, 24% (252 million pounds) for polymethylene polyphenylisocyanate, 4%(42 million pounds) for polycarbonate resins, and 11% (114 million pounds) for other chemicals, including methyl isocyanate, methylenediphenyl diisocyanate, chloroformate esters, and carbonate esters. Toluene diisocyanate is used to make polyurethane resins, which are used mostly for foams, elastomers, and coatings. Polymethylene polyphenylisocyanate is used mostly in the production of rigid polyurethane foams. Polycarbonate resin applications include appliance and electrical tool housings, electronic parts, and break-resistant glazing. Methyl isocyanate is an intermediate in the production of carbamate- (e.g., carbaryl) and urea-type pesticides. Methylenediphenyl diisocyanate is used to make polyurethane resins for adhesives, elastomers, fibers, and coatings. Chloroformate esters are used as intermediates in the production of ore-flotation agents, herbicides, insecticides, and pharmaceuticals and in perfumery. Carbonic esters (e.g., diethyl carbonate) are used as intermediates for pharmaceuticals and agricultural chemicals, as photoengraving assist agents, and as specialty solvents.

There is no substitute chemical for phosgene in these chemical intermediate applications.

Phthalic anhydride

U.S. production of phthalic anhydride was 1.02 billion pounds in 1973, 977 million pounds in 1974, and 702 million pounds in 1975. U.S. imports were 80 thousand pounds in 1973, one million pounds in 1974, and 21 million pounds in 1975. Combined U.S. exports of phthalic acid and phthalic anhydride were 23 million pounds in 1973, 34 million pounds in 1974, and 4 million pounds in 1975.

Phthalic anhydride is used exclusively as a chemical intermediate in the production of phthalate plasticizers, unsaturated polyester resins, alkyd resins, dyes, tetrachloro- and tetrabromophthalic anhydride, diallyl phthalate, polyester polyols, phenolphthalein, methyl anthranilate, and lead phthalate.

Of the 951 million pounds of phthalic anhydride consumed in the U.S. in 1974, 52% (494 million pounds) was used to make phthalate plasticizers. These are used predominantly in polyvinyl chloride plastics, and to a lesser extent in cellulose acetate, cellulose nitrate, and polyvinyl acetate.

The production of unsaturated polyester resins consumed 22% (205 million pounds) of phthalic anhydride in 1974. It functions as a modifying component to impart toughness to these resins, which are used mostly as general-purpose resins in construction, marine, and synthetic marble applications.

Alkyd resin production consumed 21% (200 million pounds) of phthalic anhydride in 1974. These resins are used in the manufacture of trade sales paints, and in industrial, marine, and maintenance finishes. The remaining 5% (52 million pounds) of phthalic anhydride consumed in 1974 was used to produce: (1) a variety of dye intermediates (consuming more than 10 million pounds of anhydride in 1974); (2) tetrabromo- and tetrachlorophthalic anhydride (fire retardant components of some polyester resins, polyurethane foams, and surface coatings); (3) diallyl phthalate (consuming about 3 million pounds of phthalic anhydride), which is chiefly used as a cross-linking agent for unsaturated polyester resins; (4) polyester polyols (polyurethane resin components); (5) phenolphthalein (mostly used as a pH indicator); (6) methyl anthranilate (a fragrance and flavor); and (7) lead phthalate (a stabilizer for polyvinyl chloride wire insulation). For the period 1974-1979, the use of phthalic anhydride is expected to have an annual average growth rate of 2-5% for plasticizer production, 10% for unsaturated polyester resin production, 1% for alkyd resin production, and 8% for all other uses, resulting in an average annual growth rate for 1974-1979 for all uses of 4.0-4.5%.

In some of the above-mentioned applications of phthalic anhydride, other chemicals are presently used. For example, isophthalic acid is used as a modifying component to impart toughness to unsaturated polyester resins. Other acids or anhydrides used in alkyd resin manufacture include maleic anhydride, isophthalic acid, and fumaric acid. There are no known substitutes for phthalic anhydride in its other intermediate uses, although other products could presumably be substituted for the phthalic anhydride-derived products.

Ketene

U.S. production of ketene in 1975 for use as a chemical intermediate in the manufacture of acetic anhydride from acetic acid is estimated to have been 665 million pounds. Ketene is available commercially as its dimer, which is also known as diketene. No data on the amount of diketene produced for non-captive uses were available. Data on U.S. imports and exports of ketene are not available.

Use as a chemical intermediate in the production of acetic anhydride from acetic acid far overshadows all of its other uses. Acetic anhydride consumption is expected to increase at less than 1% per year to 1979.

Ketene has also been used as a chemical intermediate in the production of dehydroacetic acid, acetoacetic esters, acetoacetanilide, N, N-dialkylacetoacetamides and cellulose esters which are used in the manufacture of fine chemicals, drugs, dyes, and insecticides. No data were available on the amounts of ketene used in these applications, however.

Acetic anhydride has been prepared in the past from acetylene and acetic acid in the presence of mercuric oxide, or from sodium acetate and acetyl or sulfuryl chloride, processes which do not produce ketene in an intermediate step.

Maleic anhydride

U.S. production of maleic anhydride was 290 million pounds in 1974 and 216 million pounds in 1975. A preliminary production figure of 264 million pounds has been reported for 1976. U.S. imports of maleic anhydride are estimated to have been 12 million pounds in 1974 and 5 million pounds in 1975. U.S. exports of maleic anhydride in 1975 were 925 million pounds.

The estimated U.S. consumption pattern for maleic anhydride in 1975 (all of which was used for chemical intermediate applications) was: 125 million pounds (58%) for unsaturated polyester resins; 20 million pounds (9%) for the production of agricultural chemicals; 8 million pounds (4%) for the production of fumaric acid; 6 million pounds (3%) for alkyd resins; and 57 million pounds (26%) for other chemicals.

Unsaturated polyester resins are made with glycols and unsaturated acids or anhydrides, such as maleic anhydride. When used, they are cross-linked with an unsaturated monomer such as styrene, vinyl toluene, or diallyl phthalate. Of the 771 million pounds of unsaturated polyester resins produced in 1975, 78% was used in reinforced plastic applications (e.g., marine craft and accessories, building panels, bathroom components, automobiles, and corrosion-resistant products such as tanks and pipes).

The remainder was used in non-reinforced resin applications, e.g., synthetic marble, auto repair putty, and cast furniture parts.

Agricultural chemicals derived from maleic anhydride include the insecticide malathion, the herbicides maleic hydrazide and endothall, and the fungicides captan and Difolatan®.

Most of the fumaric acid produced in the U.S. is made from maleic anhydride. However, fumaric acid is also produced by oxidizing benzene to maleic acid, which is then converted directly to fumaric acid. The largest use for fumaric acid is as a fortifier in paper size resins. It is used to a lesser extent in the production of unsaturated polyester resins, alkyd surface coating resins, plasticizers, adhesives, and lubricating oil additives, and also as a food acidulant (a declining use).

Alkyd resins derived from maleic anhydride are usually adducts of the anhydride with rosin to produce low-cost coating resins used where color retention and exterior durability are not important (e.g., metal primers, machinery and equipment enamels, and modifiers for nitrocellulose lacquers).

Maleic anhydride is used to produce many other chemicals such as: (1) polyisobutylene succinic anhydride and dodecyl succinic anhydride, used as viscosity index improvers in lubricating oils and as ashless detergent dispersants in fuels; (2) copolymers of maleic anhydride with styrene (protective colloids), ethylene (textile and paper sizes), or methyl vinyl ether (hair spray and time-release pharmaceuticals); (3) reactive plasticizers such as dibutyl maleate and dioctyl maleate, used in polyvinyl chloride and polyvinyl acetate resins; (4) malic acid, used as a food acidulant; (5) chlorendic acid and anhydride (discussed later in this Market Forecast); (6) alkyl maleates used to produce sulfosuccinate surface-active agents; and (7) small amounts of other chemicals, including succinic acid anhydride (chemical intermediate for food emulsifiers and many other products), dibutyltin maleate (plastics stabilizer), paper size resins, tetrahydrophthalic anhydride (additive for unsaturated polyester resins to increase resistance to water and solvents), and methyl tetrahydrophthalic anhydride (hardener for epoxy resins).

For the period 1974-1980, the average annual growth rate in consumption of maleic anhydride is expected to be 7.5-9.5% for unsaturated polyester resins, 6.5% for agricultural chemicals, 2% for fumaric acid, 0% for alkyd resins, 8% for lubricating additives, 6% for copolymers, 5% for reactive plasticizers, 7% for malic acid, 10% for chlorendic anhydride and acid, 5% for surface-active agents, and 2% for other chemicals. These growth rates result in an average annual growth rate for consumption of maleic anhydride for all uses of 6-7% to 1980.

In some of the above-mentioned applications of maleic anhydride, other chemicals are presently used. Fumaric acid, which can be used to make unsaturated polyester resins, can also be produced from maleic acid obtained from the oxidation of benzene. Phthalic anhydride, isophthalic acid, and fumaric acid are used to make alkyd resins. In general, it can be said that substitutes usually can be found for the final end products made from maleic anhydride, depending on economics, intended use, and performance characteristics.

Trimellitic anhydride

Because there is only one U.S. producer of trimellitic anhydride, production information is not published for proprietary reasons. However, this manufacturer is reported to have a capacity of 50 million pounds per year. Data on U.S. imports and exports are not available.

Trimellitic anhydride is used to produce trimellitate plasticizers, alkyd surface coatings, and poly(amide-imide) and poly(ester-imide) resins. The production of trimellitate plasticizers, the largest market for trimellitic anhydride, was 26 million pounds in 1974, 16 million pounds in 1975, and 1976 sales have been estimated at 30 million pounds (production data for 1976 are not yet published). These specialty plasticizers are used primarily in polyvinyl chloride (PVC) resins. This use is expected to grow at an average rate of approximately 11% per year from 1976 to 1981. An estimated 7-8 million pounds of trimellitic anhydride were consumed in 1976 for the production of alkyd (mainly water-based) and oil-free alkyd (polyester) surface coatings. The consumption of alkyd surface coatings is expected to remain constant or decline slightly over the next five years, but the consumption of water-based and oil-free alkyds is expected to increase.

An estimated 2.5 million pounds of poly(amide-imide) and poly(ester-imide) resins were produced in 1976. These resins are primarily used as wire enamels. No information was available on which to base a growth rate forecast for this application.

The choice of plasticizer depends largely on the desired properties of the plasticized products. The trimellitates are used primarily where good performance over a wide temperature range is necessary, such as in wire insulation and some automotive applications. Other plasticizers used in PVC resins include phthalates, epoxy esters, phosphate esters, aliphatic esters, and linear polyesters. Of these, the linear polyesters, the so-called polymeric plasticizers, are frequently used for their permanence but lack the low temperature properties of the trimellitates.

Other polybasic acids suggested for use in water-based alkyds include 2,2-bis(hydroxymethyl)propionic acid and pentanetricarboxylic acid.

Straight and unsaturated polyimide resins, derived from the tetrafunctional anhydrides, pyromellitic dianhydride and benzophenone tetracarboxylic dianhydride, are also used as wire enamels.

Benzoyl chloride

The U.S. production of benzoyl chloride in 1974 is estimated to have been 18.6 million pounds. Data on U.S. imports and exports are not available.

Approximately 10.6 million pounds of benzoyl chloride (57% of total 1974 production) was used in the production of benzoyl peroxide, an initiator and cross-linking agent used in the manufacture of a variety of polymers. An estimated 7.2 million pounds (39%) were used to produce herbicides, the most important of which is amiben (3-amino-2,5-dichlorobenzoic acid). Approximately 600 thousand pounds (3%) were used as a dye intermediate in the manufacture of Mordant Brown 44 and anthraquinone dyes. The remaining 200 thousand pounds (1%) were consumed as an intermediate for plasticizers and drugs. No information was available on which to base a market forecast for benzoyl chloride.

There are no known substitutes for benzoyl chloride in the above-mentioned intermediate applications. (For a discussion of polymerization initiators, see the Market Forecast on benzoyl peroxide.)

Tetrachloro- and tetrabromophthalic anhydride

The combined U.S. production of tetrachloro- and tetrabromophthalic anhydride in 1973 is estimated to have been 10-15 million pounds. Data on U.S. imports and exports are not available.

Tetrachloro- and tetrabromophthalic anhydride are used as components of some unsaturated polyester resins, polyurethane foams, and surface coatings because they impart fire retardancy to the polymer. Unsaturated polyester resins consumed an estimated 2 million pounds of these halogenated anhydrides in 1976. No data have been found as to the relative amounts of these anhydrides consumed in polyurethane foams or surface coatings. Flame-retarded unsaturated polyester resins have a number of end uses, including marine, construction, and transportation applications, and in consumer goods, corrosion-resistant products (e.g., tanks and pipes), electrical components, and miscellaneous fiber-reinforced products. No data are available on which to base a market forecast for these anhydrides. The average annual growth rate to 1980 for unsaturated polyester resins is estimated to be 9.4-12% for all uses. With the continuing emphasis on fire retardance, the use of these fire-retardant components will undoubtedly keep pace with the growth of the resin market.

Chlorendic anhydride, dibromobutenediol, and dibromopropyl methacrylate are also presently used to impart flame retardancy to unsaturated polyester resins. One manufacturer has a series of brominated resins prepared by a proprietary bromination process which have a low flame spread and low smoke density.

Chlorendic anhydride

The combined U.S. production of chlorendic anhydride and chlorendic acid in 1974 is estimated to have been 10 million pounds. Data on U.S. imports and exports are not available.

The principal use of chlorendic acid and anhydride is in the manufacture of unsaturated polyester resins with fire retardant properties. These resins are used in marine, construction, transportation, corrosion-resistant, and fiber-reinforced applications. Smaller amounts are consumed in alkyd resins used in fire-resistant paints for military applications and as a hardener for epoxy resins. No data as to relative amounts for these applications are available.

The average annual growth rate to 1980 for consumption of unsaturated polyester resins is expected to be 8-10% for marine applications, 10-12% for construction, 10-16% in transportation, 16-18% in corrosion resistant products, and 6-8% in fiber-reinforced resin applications, with a resultant average growth rate of 10-12% for unsaturated polyester resins in which chlorendic acid or anhydride is a component.

Other acid components in unsaturated polyester resins used to impart fire retardancy include tetrachlorophthalic anhydride and tetrabromophthalic anhydride or additive flame retardants such as triethyl phosphate in conjunction with alumina trihydrate.

Other acids presently used in alkyd resin surface coatings to impart flame retardancy include tetrachlorophthalic anhydride. The type of curing agent used in epoxy resins depends on the type of resin used and on the particular application for the cured resin. Other anhydrides used include phthalic anhydride, tetrahydrophthalic anhydride, and pyromellitic dianhydride.

Lauroyl chloride

The U.S. production of lauroyl chloride in recent years has been: 4.2 million pounds in 1973, 2.3 million pounds in 1974, and 1.4 million pounds in 1975. Data on U.S. imports and exports are not available.

Lauroyl chloride is used principally as a chemical intermediate in the manufacture of lauroyl peroxide and in the manufacture of lauroyl sarcosines. Lauroyl peroxide is used as a free-radical initiator in vinyl-type polymerizations. The lauroyl sarcosines are used in a variety of detergent and emulsifier applications, such as in dentifrices; in shampoos; in rug, upholstery, and window cleaners; and in emulsion polymerizations. The production of lauroyl chloride has declined somewhat in recent years, but no information was available to determine if this trend will continue.

Other free radical initiators presently used by the polymer industry include other peroxides (such as benzoyl peroxide or di-tert-butyl peroxide) and azo compounds. In the formulating of detergent compositions, many different products are available with similar properties. The choice of substitutes for the lauroyl sarcosines would require a highly-skilled expert and would depend on factors such as cost, availability of raw materials, intended applications, and performance.

ACYLATING AGENTS WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
108247	Acetic anhydride	1458×10^6 lbs./1975/T75	25 (delivered)	365	I
75445	Phosgene	796×10^6 lbs./1975/T75	25 (works)	200	--
85449	Phthalic anhydride	702×10^6 lbs./1975/T75	25.5 (f.o.b., East Coast)	179	I
463514	Ketene	665×10^6 lbs./1975/SRI (as intermediate)	--	--	--
108316	Maleic anhydride	216×10^6 lbs./1975/T75	37 (works, frt. eqlzd.)	80	I, II
552307	Trimellitic anhydride	50×10^6 lbs./1976/SRI (capacity)	--	--	--
98884	Benzoyl chloride	18.6×10^6 lbs./1974/SRI	52 (works)	10	--
117088	Tetrachlorophthalic anhydride }	$15-20\times10^6$ lbs./1973/SRI	--	--	--
632791	Tetrabromophthalic anhydride }				
115275	1,4,5,6,7,7-Hexachloro-5-norbornene-2,3-dicarboxylic anhydride (chlorendic anhydride)	10×10^6 lbs./1974/SRI (includes chlorendic acid)	35 (works)	3.5	--
112163	Lauroyl chloride	1.4×10^6 lbs./1975/T75	--	--	--

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*Taken from Chemical Marketing Reporter, April 11, 1977, reflecting the list prices prevailing for large lots.

Class: Acylating Agents

ACYLATING AGENTS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
541413	Carbonochloridic acid, ethyl ester (Ethyl chloroformate)	887x10^3 lbs./1975/T75 (sales)
99638	Isophthaloyl chloride	<6x10^5 lbs./1974/SRI
75365	Acetyl chloride	>1000 lbs./1977/SRI (Stage I dossier)
76028	Trichloroacetyl chloride	>1000 lbs./1977/SRI
79038	Propionyl chloride	>1000 lbs./1975/T75
79049	Chloroacetyl chloride	>1000 lbs./1975/T75
79221	Chloroformic acid, methyl ester (Methyl chloroformate)	>1000 lbs./1977/SRI
79301	Isobutyryl chloride	>1000 lbs./1975/T75
79378	Oxalyl chloride	>1000 lbs./1977/SRI
81083	o-Sulfobenzoic acid, cyclic anhydride	>1000 lbs./1975/T75
81845	1,8-Naphthalic anhydride	>1000 lbs./1975/T75
83012	Diphenylcarbamoyl chloride	>1000 lbs./1977/SRI
85427	1,2-Cyclohexanedicarboxylic anhydride	>1000 lbs./1975/T75
88108	Diethylcarbamoyl chloride	>1000 lbs./1977/SRI
88959	Phthaloyl chloride	>1000 lbs./1975/T75
89327	1,2,4,5-Benzenetetracarboxylic-1,2:4,5-dianhydride	>1000 lbs./1975/T75
89758	2,4-Dichlorobenzoyl chloride	>1000 lbs./1975/T75

Class: Acylating Agents

ACYLATING AGENTS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source	
97723	Isobutyric anhydride	>1000 lbs./1975/T75	
99332	3,5-Dinitrobenzoyl chloride	>1000 lbs./1975/T75	
100072	p-Anisoyl chloride	>1000 lbs./1977/SRI	
100209	Terephthaloyl chloride	>1000 lbs./1975/T75	
102921	Cinnamoyl chloride	>1000 lbs./1975/T75	
103800	Phenylacetyl chloride	>1000 lbs./1977/SRI	
106310	Butyric anhydride	>1000 lbs./1975/T75	
108236	Chloroformic acid, isopropyl ester (Isopropyl chloroformate)	>1000 lbs./1975/T75	
108305	Succinic anhydride	>1000 lbs./1975/T75	(Stage I and II dossiers)
108554	Glutaric anhydride	>1000 lbs./1975/T75	
111193	Sebacoyl chloride	>1000 lbs./1975/T75	
111502	Adipoyl chloride	>1000 lbs./1977/SRI	
111648	Octanoyl chloride	>1000 lbs./1975/T75	
112130	Decanoyl chloride	>1000 lbs./1975/T75	
112674	Palmitoyl chloride	>1000 lbs./1975/T75	
112765	Stearoyl chloride	>1000 lbs./1975/T75	
112776	Oleoyl chloride	>1000 lbs./1975/T75	

Class: Acylating Agents

ACYLATING AGENTS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
117408	5-Methyl-5-norbornene-2,3-dicarboxylic anhydride	>1000 lbs./1975/T75
121904	m-Nitrobenzoyl chloride	>1000 lbs./1977/SRI
122010	p-Chlorobenzoyl chloride	>1000 lbs./1975/T75
123626	Propionic anhydride	>1000 lbs./1975/T75
141753	Butyryl chloride	>1000 lbs./1977/SRI
354325	Trifluoroacetyl chloride	>1000 lbs./1977/SRI
501531	Chloroformic acid, benzyl ester (Benzyl chloroformate)	>1000 lbs./1977/SRI
506967	Acetyl bromide	>1000 lbs./1977/SRI
598210	Bromoacetyl bromide	>1000 lbs./1975/T75
609654	o-Chlorobenzoyl chloride	>1000 lbs./1975/T75
616024	Citraconic anhydride	>1000 lbs./1975/T75
618462	m-Chlorobenzoyl chloride	>1000 lbs./1977/SRI
641703	3-Nitrophthalic anhydride	>1000 lbs./1975/T75
674828	Diketene (Ketene dimer) (2-Oxetanone,4-methylene-)	>1000 lbs./1975/T75

Class: Acylating Agents

ACYLATING AGENTS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
760678	2-Ethylhexanoyl chloride	>1000 lbs./1975/T75
1204280	Trimellitic anhydride, acid chloride	>1000 lbs./1975/T75
1885149	Carbonochloridic acid, phenyl ester (Phenyl chloroformate)	>1000 lbs./1977/SRI
1989533	2,6-Dimethoxybenzoyl chloride	>1000 lbs./1975/T75
2094726	1-Adamantanecarboxylic acid chloride	>1000 lbs./1977/SRI
2561855	Dodecyl succinic anhydride	>1000 lbs./1975/T75
2936085	Di-n-propylacetic acid chloride (and acid)	>1000 lbs./1975/T75
3282302	Propanoyl chloride,2,2-dimethyl- (Pivaloyl chloride)	>1000 lbs./1975/T75
4462559	3-(2',6'-Dichlorophenyl)-5-methyl-4-isoxazole-4-carbonyl chloride	>1000 lbs./1975/T75
7144083	Cholest-5-en-3-ol (3.beta.)-, carbonochloridate (Cholesteryl chloroformate)	>1000 lbs./1977/SRI
10328924	N-Methyl-N-carboxyanthranilic anhydride	>1000 lbs./1975/T75
16883162	3-Phenyl-5-methylisoxazole-4-carbonyl chloride	>1000 lbs./1975/T75
18310606	2-Methyl-5-norbornene-2,3-dicarboxylic anhydride	>1000 lbs./1975/T75
18956871	10H-Phenothiazine-10-carbonyl chloride	>1000 lbs./1977/SRI
25377735	Dodecenylsuccinic anhydride	>1000 lbs./1975/T75

Class: Acylating Agents

ACYLATING AGENTS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
25629509	3-(o-Chlorophenyl)-5-methyl-4-isoxazole carbonylchloride	>1000 lbs./1975/T75
26680546	Octenylsuccinic anhydride	>1000 lbs./1975/T75
28928974	Nonenylsuccinic anhydride	>1000 lbs./1975/T75
32072961	n-Hexadecenylsuccinic anhydride	>1000 lbs./1975/T75
39098970	Thiopheneacetyl chloride	>1000 lbs./1975/T75
40292828	Neodecanoyl chloride (2,2-Dimethyloctanoyl chloride)	>1000 lbs./1975/T75
55150293	2-Ethoxy-1-naphthoyl chloride	>1000 lbs./1975/T75

Class: Acylating Agents

ACYLATING AGENTS WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
79447	Dimethylcarbamoyl chloride
93970	Benzoic anhydride
122043	p-Nitrobenzoyl chloride
507028	Acetyl iodide
557993	Acetyl fluoride
678773	Perfluoroglutaryl chloride
879185	1-Naphthalenecarbonyl chloride
2528612	Heptanoyl chloride

3. Class III: Peroxides

The ten chemicals in this group are those with a known or estimated annual U.S. production level of one million pounds or more. They can be divided into two groups based on their major use classification: (1) the three peroxides that are not used primarily as polymerization initiators but as industrial chemicals; and (2) the remaining seven peroxides that are used chiefly as polymerization initiators.

Industrial Chemicals

This subset includes the three peroxides that account for more than 99% of the total annual production of all ten peroxides represented in the class: cumene hydroperoxide, hydrogen peroxide, and peroxyacetic acid. Because they have use patterns which apply for the most part to the chemical rather than to the subset, the chemicals will be discussed individually.

Cumene hydroperoxide

U.S. production figures for cumeme hydroperoxide are not available. However, the amount of cumene hydroperoxide produced and consumed captively in the manufacture of phenol and acetone from cumene is estimated to have been 2256 million pounds in 1975 and 3178 million pounds in 1976.

During 1976-1981, demand for cumene hydroperoxide as an unisolated intermediate in phenol/acetone manufacture is expected to grow at an average annual rate of 7-8% per year.

Phenol can also be made by the benzene sulfonation process, the chlorobenzene process, and the toluene oxidation process. Acetone is primarily produced by the catalytic dehydrogenation of isopropyl alcohol. Acetone may also be produced by the oxidation of isopropyl alcohol with oxygen and by various other processes where it is obtained as a by-product.

A small amount of cumene hydroperoxide is also produced for use as an intiator for acrylic resins polymerization and as a curing agent for unsaturated polyester resins. (Further information on the use of peroxides as initiators and curing agents for polymers is discussed later in this report.)

Hydrogen peroxide

U.S. production of hydrogen peroxide amounted to 155 million pounds (100% by weight) in 1975. U.S. imports amounted to 2.4 million pounds. Data on U.S. exports of hydrogen peroxide are not available.

U.S. demand for hydrogen peroxide is expected to grow by at least 5% per year to 1980.

The estimated U.S. consumption pattern for hydrogen peroxide in 1976 is as follows: textile bleaching, 30%; synthesis of perborates, plasticizers, and other chemicals, 28%; synthesis of glycerin, 8%; pulp and paper, 8%; water treatment, 5%; and miscellaneous applications, 21%.

Hydrogen peroxide is used in about 85-90% of all cotton bleaching processes in the U.S. as well as for bleaching cotton blends.

Hypochlorite bleaches, competitors of hydrogen peroxide, are also used in textile bleaching.

Hydrogen peroxide is used to produce household laundry perborate bleaches; in the production of epoxidized vegetable oils and fatty acid esters (used mainly as PVC stabilizers and plasticizers); and to manufacture other chemicals including peracids, and organic and inorganic peroxides. These end-use markets are not expected to grow significantly during the next few years.

Only one U.S. chemical plant produces synthetic glycerin from allyl alcohol and hydrogen peroxide. Most synthetic glycerin is produced by the allyl chloride-epichlorohydrin process, but can also be produced from allyl alcohol and peracetic acid via glycidol. Synthetic glycerin production from hydrogen peroxide is not expected to increase significantly.

The pulp and paper industry uses hydrogen peroxide to bleach groundwood pulp and, to a lesser extent, in the final bleaching stages of chemical pulps. If hydrogen peroxide were used to replace some of the chlorine and sodium chlorate used in pulp bleaching, possible market growth potential would be significant. Another potential market for increased hydrogen peroxide demand in this industry is de-inking newsprint from recycling operations.

Waste water treatment represents the fastest growing market for hydrogen peroxide consumption. Producers expect water treatment to become the third largest end-use market for hydrogen peroxide (consuming 20 million pounds per year) by 1980. Chlorine is the major competitor in this area, and ozone is also used.

Miscellaneous applications for hydrogen peroxide include its use in cosmetics; fruit juice and food bleaching; wax, oil, and wood bleaching; and rocket fuel. A potential application is its use as an oxidizing agent in the in-situ leaching of uranium ores.

Peroxyacetic acid

U.S. production figures for peroxyacetic acid are not reported. U.S. plant capacity for the production of peroxyacetic acid is believed to be greater than 150 million pounds per year. Data on U.S. imports and exports of peroxyacetic acid are not available.

Most of the peroxyacetic acid produced in the U.S. is consumed in situ for the production of epoxides from unsaturated materials, e.g., epoxidized soybean oils and fatty esters, styrene oxide, and vinylcyclohexene dioxide. Epoxidized soybean oils and fatty esters are used as stabilizers and plasticizers for polyvinyl chloride resins. Epoxidized soybean oil demand is expected to grow at an average annual rate of 6.4% per year during the next five years.

Peroxyacetic acid is also consumed captively in the manufacture of synthetic glycerin. However, less than 13% of the total U.S. synthetic glycerin production capacity is contributed by the allyl alcohol-peracetic acid-glycidol route. Most synthetic glycerin is produced in the U.S. by the allyl chloride-epichlorohydrin route.

Peroxyacetic acid is also used in bleaching textile fibers (including cellulose, acetate rayon, polyamide, polyesters, and blends); pulp and paper; fats, oils and waxes; and glue and starch. It is also used as a polymerization catalyst; as an oxidizing agent in organic synthesis; as a sterilizing agent in food processing; and as a fungicide used on baskets, bins, lugs, storage room surfaces, and other containers used in harvesting crops.

Polymerization Initiators

Since the remaining seven peroxides, benzoyl peroxide, methyl ethyl ketone peroxide, di-tert-butyl peroxide, tert-butyl peroxybenzoate, lauroyl peroxide, tert-butylperoxy-2-ethylhexanoate, and tert-butyl peroxypivalate, are all used primarily as polymerization initiators, they will be discussed as a group.

About seventy organic peroxides are used in the plastics industry--primarily as polymerization initiators for acrylic resins, polyethylene, polystyrene, and polyvinyl chloride resin production. Another important use is in the curing of unsaturated polyesters, as well as crosslinking agents for high and low density polyethylenes and for natural and synthetic rubbers (e.g., silicone).

Process conditions and the specific properties desired in the end product may require mixtures of several peroxides or certain peroxides which are generally not commonly used for the polymer. The choice of a specific organic peroxide for a given reaction depends on the temperature at which the chemical reaction takes place and on the rate of decomposition of the peroxide.

The table below lists the 1974 and 1975 U.S. production figures for the seven organic peroxides under consideration. Production figures reported in 1975 are significantly below the 1974 production figures which were apparently the highest in recent years. Demand for organic peroxides in 1976 was expected to have returned to 1974 levels.

Exports data are not available for these peroxides.

	Annual Production (Millions of Pounds)	
	1975	1974
Benzoyl peroxide	7.9*	9.1
Methyl ethyl ketone peroxide	6.4	6.7
Di-tert-butyl peroxide	2.3	3.0
tert-Butyl peroxybenzoate	2.2	2.7
Lauroyl peroxide	1.3†	1.7†
tert-Butylperoxy-2-ethylhexanoate	1.2	1.6
tert-Butyl peroxypivalate	1.03	---

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*U.S. Imports of benzoyl peroxide through principal U.S. customs districts in 1975 totaled 100 thousand pounds.

†Consumption estimate

The future outlook for organic peroxides is linked to the demand for the various plastics in their end-use markets.

Three of the seven peroxides under consideration have other minor uses. Benzoyl peroxide is also used as a bleaching agent for fats, oils, waxes, and flour; as a drying agent for unsaturated oils; as a burn-out agent for acetate yarns; as a keratolytic agent in pharmaceutical and cosmetic products; and in cheese manufacture.

Di-tert-butyl peroxide also has reported use as an ignition accelerator for diesel fuels and in organic synthesis.

Lauroyl peroxide is also used as a bleaching agent; as a drying agent for fats, oils, and waxes; and as a chemical intermediate.

Class: Peroxides

PEROXIDES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
80159	Cumene hydroperoxide (α,α-dimethylbenzyl hydroperoxide)	3062x10^6 lbs./1977/SRI	--	--	--
7722841	Hydrogen peroxide	160x10^6 lbs.(100%)/1975/SRI	15.5 (35% soln.) (frt. eqlzd.)	71	--
79210	Peroxyacetic acid	150x10^6 lbs./1973/SRI (capacity)	--	--	I, II
94360	Benzoyl peroxide	7.9x10^6 lbs./1975/T75	190 (works, frt. eqlzd.)	15	I
--	Methyl ethyl ketone peroxide (2-Butanone peroxide)	6.4x10^6 lbs./1975/T75	95 (T75)	6.1	--
110054	Di-tert-butyl peroxide	2.3x10^6 lbs./1975/T75	94 (T75)	2.2	--
614459	tert-Butyl peroxybenzoate	2.2x10^6 lbs./1975/T75	159 (T75)	3.5	--
105748	Lauroyl peroxide	1.5x10^6 lbs./1976/SRI (consumption)	--	--	--
3006824	tert-Butylperoxy-2-ethylhexanoate	1.2x10^6 lbs./1975/T75	214 (T75)	2.6	--
927071	tert-Butyl peroxypivalate	1.03x10^6 lbs./1975/T75	253 (T75	2.6	--

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*Taken from Chemical Marketing Reporter, April 11, 1977, reflecting the list prices prevailing for large lots. Values designated as coming from Synthetic Organic Chemicals, United States Production and Sales (T75), are unit sales value which is calculated from total quantities sold (the sum of the large quantities sold on a contractual basis and smaller quantities sold intermittently) and total sales value (the sum of the values of sales at contract prices and list prices).

Class: Peroxides

PEROXIDES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
762129	Didecanoyl peroxide	$275x10^3$ lbs./1976/SRI (consumption)
75912	tert-Butyl hydroperoxide	>1000 lbs./1975/T75
78182	1-Hydroperoxycyclohexyl 1-hydroxycyclohexyl peroxide (cyclohexanone peroxide)	>1000 lbs./1975/T75
78637	(1,1,4,4-Tetramethyltetramethylene)bis(tert-butyl peroxide) (2,5-dimethyl-2,5-bis(tert-butylperoxy)hexane)	>1000 lbs./1975/T75
80433	Bis(α,α-dimethylbenzyl)peroxide (dicumyl peroxide)	>1000 lbs./1977/SRI
80477	p-Menth-8-yl hydroperoxide	>1000 lbs./1975/T75
105646	Peroxydicarbonic acid, diisopropyl ester (diisopropylperoxydicarbonate)	>1000 lbs./1975/T75
107711	tert-Butyl peroxyacetate	>1000 lbs./1975/T75
109137	tert-Butyl peroxyisobutyrate	>1000 lbs./1975/T75
110225	Diacetyl peroxide	>1000 lbs./1975/T75
123239	Succinic acid peroxide	>1000 lbs./1975/T75
133142	Bis(2,4-dichlorobenzoyl)peroxide	>1000 lbs./1975/T75
1068275	2,5-Dimethyl-2,5-di(tert-butylperoxy)hexyne-3	>1000 lbs./1975/T75
1931620	OO-tert-Butyl hydrogen monoperoxymaleate (tert-Butylperoxymaleic acid)	>1000 lbs./1975/T75

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Class: Peroxides

PEROXIDES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
2212819	1,3-Bis(tert-butylperoxyisopropyl)benzene	>1000 lbs./1977/SRI
2372216	Carbonoperoxoic acid, OO-(1,1-dimethylethyl) O-(1-methylethyl) ester (tert-Butylperoxyisopropyl carbonate)	>1000 lbs./1975/T75
2618771	2,5-Bis(benzoylperoxy)-2,5-dimethylhexane	>1000 lbs./1975/T75
3025885	2,5-Dimethylhexane-2,5-dihydroperoxide	>1000 lbs./1977/SRI
3179564	Acetylcyclohexanesulfonyl peroxide	>1000 lbs./1975/T75
5809085	1,1,3,3-Tetramethylbutyl hydroperoxide	>1000 lbs./1975/T75
6731368	1,1-tert-Butylperoxy-3,3,5-trimethylcyclohexane	>1000 lbs./1977/SRI
13052067	2,5-Dimethylhexane-2,5-diperoxyoctoate	>1000 lbs./1975/T75
13052090	2,5-Dimethyl-2,5-bis(2-ethyl-1-hexanoylperoxy)hexane	>1000 lbs./1975/T75
16066389	Di-n-propyl peroxydicarbonate	>1000 lbs./1975/T75
16111629	Di(2-ethyl-1-hexyl)peroxydicarbonate	>1000 lbs./1975/T75
19910657	Di-sec-butylperoxydicarbonate	>1000 lbs./1975/T75
26748414	tert-Butyl peroxyneodecanoate	>1000 lbs./1975/T75
26762936	Diisopropyl benzene hydroperoxide	>1000 lbs./1975/T75

Class: Peroxides

PEROXIDES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
2407945	Bis(1-hydroxycyclohexyl)peroxide
13020069	1-Methylpropylhydroperoxide

4. Class IV: Halogenated Hydrocarbons and Derivatives

a. Class IVA: Halogenated Unsaturated Hydrocarbons

There are eight members of this class with an annual U.S. production greater than one million pounds. However, two of these chemicals, chlordane and heptachlor, are used almost exclusively as pesticides and will not be discussed further. Because the remaining six chemicals have different use patterns, they will be discussed individually.

Vinyl chloride

U.S. production of vinyl chloride in recent years has been as follows (billions of pounds): 1974 - 5.62; 1975 - 4.20; and 1976 - 5.74. U.S. imports of vinyl chloride have been less than 5 million pounds per year in recent years. U.S. exports were above 600 million pounds in 1970-1972, dropped to 410-420 million pounds in 1973-1975, and are believed to have increased to approximately 630 million pounds in 1976.

Approximately 85% of 1976 vinyl chloride consumption was used in the manufacture of polyvinyl chloride homopolymer and copolymer resins (PVC resins), 11% was exported, and the remaining 4% was used for miscellaneous other uses, including captive consumption for the synthesis of methyl chloroform and as a comonomer in the manufacture of vinylidine chloride copolymers.

There are no substitutes for vinyl chloride as the monomer for producing PVC resins. Future growth in production of vinyl chloride will be largely dependent on the growth in demand for these PVC resins. This demand is expected to increase at an average annual rate of 8-10% through 1981, with expected increased usage in construction applications (e.g., pipe and conduit) making the major contribution. Although numerous other resins compete with PVC resins in the variety of markets which they presently have, very few combine the low cost and performance features of PVC resins, particularly in the major markets for PVC resins--construction, consumer goods, packaging, and electrical uses.

Tetrachloroethylene

U.S. production of this chemical (which is also known as perchloroethylene) in recent years has been as follows (millions of pounds): 1974 - 734; 1975 - 679; 1976 - 657. U.S. imports of tetrachloroethylene amounted to 37.5 million pounds in 1975 and 62 million pounds in 1976. Exports totaled 52.6 million pounds in 1975.

The U.S. domestic consumption pattern for tetrachloroethylene in 1974 was: uses in dry cleaning and in textile processing and finishing, 69%; use in metal cleaning, 16%; use as a chemical intermediate for the synthesis of fluorocarbons (113, 114, 115, and 116), 12%; and miscellaneous uses (e.g., as a solvent for silicones and for aerosol pre-laundry garment sprays), 3%.

In mid-1976, growth in U.S. consumption of tetrachloroethylene through 1979 was expected to increase at an average annual rate of 3-4% with metal cleaning and intermediate uses accounting for most of this rate of growth. However, since then, NIOSH has recommended a lower standard for occupational exposure to tetrachloroethylene, the National Cancer Institute

(NCI) has found that orally administered tetrachloroethylene causes liver tumors in mice, and several government agencies have either banned the use of fluorocarbons in some products, have taken steps to limit their use in other products, or are moving toward banning them in still more of their major application areas. In the light of all these developments, it seems likely that earlier market forecasts will not prove correct and that reduction in the use of tetrachloroethylene in all of its applications is more likely in the future.

In dry cleaning operations, hydrocarbon solvents (e.g., Stoddard solvent) are the major tetrachloroethylene competitors, but 1,1,2-trichloro-1,2,2-trifluoroethane (Fluorocarbon 113), a derivative of tetrachloroethylene, has found some use, particularly in coin-operated equipment, in recent years, in spite of its cost. In metal cleaning, both trichloroethylene and 1,1,1-trichloroethane (methyl chloroform) have been the tranditional competitors with selection based upon their properties and the cleaning system used. NCI findings that trichloroethylene causes tumors in mice and NIOSH recommendations for lower occupational standards for trichloroethylene point to 1,1,1-trichloroethane becoming the major metal cleaning solvent, but not completely displacing the others.

2-Chloro-1,3-butadiene

U.S. production of this chemical (which is also known as chloroprene) is estimated to have been about 400 million pounds in 1974 and approximately 350 million pounds in 1975. U.S. imports and exports are believed to be negligible.

All U.S. production of polychloroprene (neoprene) elastomers is based on the use of butadiene as the raw material. Chlorination produces a mixture of dichlorobutenes from which 3,4-dichloro-1-butene is isolated.

This is dehydrochlorinated with aqueous sodium hydroxide to 2-chloro-1,3-butadiene, which is polymerized to the elastomers. The intermediate 2-chloro-1,3-butadiene appears to be used exclusively for production of these elastomers.

The estimated U.S. domestic consumption pattern for polychloroprene elastomers in 1975 was: industrial rubber goods (belts, hose, gaskets), 35%; automotive applications (hose, belts, weather stripping), 28%; wire and cable, 13%; construction (seals, gaskets), 10%; adhesives, 8%; and other uses, 6%. The average annual growth rate for polychloroprene elastomers is expected to be about 4% through 1981.

There are no substitutes for 2-chloro-1,3-butadiene as the monomer for producing polychloroprene elastomers. Polychloroprene is used in a wide variety of applications, in spite of its high price, primarily because of its outstanding resistance to weathering or combinations of deteriorating effects (e.g., abrasion, heat, solvents). Although many other elastomers compete with them successfully in some areas because of better cost-effectiveness, polychloroprene elastomers effectively have no substitutes in many of their applications. An authoritative listing of the most likely candidate substitutes for these uses could only be made by an expert in rubber technology.

Trichloroethylene

U.S. production of trichloroethylene in recent years has been as follows (million of pounds): 1974 - 388; 1975 - 293; and 1976 - 303. U.S. imports amounted to 8.4 million pounds in 1975 and 15.6 million pounds in 1976. Exports totaled 34 million pounds in 1975.

The U.S. domestic consumption pattern for trichloroethylene in 1974 was: use in metal cleaning, 90%; miscellaneous solvent and chemical intermediate uses, 10%. In late 1975, U.S. consumption of trichloroethylene was expected to decrease at an average annual rate of about 1% in spite of an expected increase in use in metal cleaning. Since then OSHA has recommended a lower standard for occupational exposure to trichloroethylene, the NCI has found that trichloroethylene causes tumors in mice, and the Food and Drug Administration has moved toward banning the use of trichloroethylene in foods, drugs, and cosmetics. In the light of these developments, it seems likely that the rate of decline in consumption will be greater than predicted earlier.

In metal cleaning, both tetrachloroethylene (perchloroethylene) and 1,1,1-trichloroethane (methyl chloroform) have been the traditional competitors with selection based upon their properties and the cleaning system used. As described under Tetrachloroethylene, a number of recent developments concerning tetrachloroethylene point to 1,1,1-trichloroethane becoming the major metal cleaning solvent, but not completely displacing the others.

1,1-Dichloroethylene

U.S. production of this chemical (which is also known as vinylidene chloride) as an isolated chemical is estimated to have been 170 million pounds annually in the years 1973-1975. It is also produced as an unisolated intermediate for hydrochlorination to 1,1,1-trichloroethane (methyl chloroform) and an estimated 100-110 million pounds was produced for this purpose in 1974. Data on U.S. imports and exports of 1,1-dichloroethylene are not available but the quantity imported and exported is believed to be negligible.

Excluding the 1,1-dichloroethylene used for 1,1,1-trichloroethane production, the estimated U.S. consumption pattern in 1974 was: use in manufacture of copolymer resins, over 90%; other uses (primarily use as a comonomer in modacrylic fibers), less than 10%.

Although copolymers of 1,1-dichloroethylene with acrylonitrile or alkyl acrylates are believed to be produced commercially, the most important copolymers are those with vinyl chloride. These copolymers are available in a variety of forms for use in a range of applications where their resistance to the effects of water vapor and chemicals is important. Included are extruded films and lacquer resins (both of which are used widely in food packaging), latexes (used as paper and plastics coatings), and extruded fibers and monofilaments (used in applications where resistance to weathering or chemicals is required).

An estimated 11-16 million pounds of 1,1-dichloroethylene was used in 1974 as a comonomer in the production of modacrylic fibers. The most important of these fibers is believed to be based on a copolymer containing 37% acrylonitrile, 40% 1,1-dichloroethylene, and lesser amounts of other monomers. The 1,1-dichloroethylene is used to increase the fire resistance of these copolymers over that of the acrylic resins (>85% acrylonitrile content) used for acrylic fibers.

In 1975, one company was reported to be considering the use of 1,1-dichloroethylene for the synthesis of monochloroacetyl chloride starting in 1976. Whether this was done or not is not known.

In late 1975, U.S. production of 1,1-dichloroethylene as an isolated chemical was expected to increase at an average annual rate of 7% through 1979. Any such growth will largely be dependent on the growth of the

1,1-dichloroethylene copolymer resins. There are no substitutes for 1,1-dichloroethylene as the principal monomer used in the production of these resins. One of the major uses of these resins appears to be in food packaging, and--at present--there are conflicting reports about the potential carcinogenic hazard posed by residual 1,1-dichloroethylene in such food packaging. Consequently, it is impossible to predict whether this market for the resins will be adversely affected.

The production of 1,1-dichloroethylene as an unisolated intermediate for use in one of the methods of synthesis of 1,1,1-trichloroethane may show a significant increase in the future. This is based on the belief (discussed under Tetrachloroethylene and Trichloroethylene) that 1,1,1-trichloroethane may become the major metal cleaning solvent.

In late 1975, U.S. consumption of modacrylic fibers, which find use in apparel (largely for deep pile fabrics with fur-like feel and appearance) and home furnishings (e.g., in fire resistant carpets), was expected to increase at an average annual rate of as much as 9% per year. In recent months, the possible carcinogenicity of the principal comonomer that is used in modacrylic fibers, acrylonitrile, has been reported. It is too soon to evaluate whether this will have an adverse effect on this market for 1,1-dichloroethylene. Other comonomers (e.g., vinyl bromide finds some use) could be used (probably at higher cost) to replace 1,1-dichloroethylene as the monomer contributing increased flame resistance to these modacrylic fibers.

Tetrafluoroethylene

U.S. production of tetrafluoroethylene was 24.6 million pounds in 1974 and 17.3 million pounds in 1975. Data on U.S. imports and exports are not available.

Use as a monomer in the production of polytetrafluoroethylene resins is believed to be by far the most important use of tetrafluoroethylene. It is also used as a comonomer in the production of several other fluorocarbon resins: fluorinated ethylene-propylene, poly (ethylene-tetrafluoroethylene), perfluoroalkoxy, and poly (vinylidene fluoride-hexafluoropropylene-tetrafluoroethylene). Another fluorocarbon monomer, hexafluoropropylene, can also be produced by the pyrolysis of tetrafluoroethylene but it may be produced commercially as a by-product of the pyrolysis of chlorodifluoromethane to produce tetrafluoroethylene.

The estimated U.S. consumption pattern for polytetrafluoroethylene resins in 1975 was: 36% in chemical applications (e.g., valves, linings, packings), 25% in mechanical applications (seals and piston rings), 20% in electrical uses (insulation and tape), and 19% in other applications (consumer cookware, industrial coatings, and lubricants).

There are no substitutes for tetrafluoroethylene as the monomer for producing polytetrafluoroethylene resins. These expensive resins find use in a variety of specialty applications because of their outstanding combination of properties such as chemical resistance, low coefficient of friction, excellent dielectric properties, and good weatherability. They compete with other engineering plastics (e.g., nylon) and with high performance plastics (e.g., polyimides) and the choice is made on a cost-effectiveness basis.

U.S. production of polytetrafluoroethylene resins dropped sharply in 1975. However,U.S. consumption of polytetrafluoroethylene resins is expected to grow at an average annual rate of 6% until 1980 with aqueous dispersions providing the greatest part of the growth.

Revised 8/77

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Unsaturated Hydrocarbons

HALOGENATED UNSATURATED HYDROCARBONS WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*,¢/lb.	Market Value, Million $	Dossiers
75014	Vinyl chloride	5736.5x10^6 lbs./1976/T76	14 (f.o.b. works)	587.5	I, II
127184	Tetrachloroethylene (Perchloroethylene)	657.2x10^6 lbs./1976/T76	16 (distr., dlvd.)	108.7	IA
126998	2-Chloro-1,3-butadiene (Chloroprene)	349x10^6 lbs./1975/SRI	--	--	I, II
79016	Trichloroethylene	303.3x10^6 lbs./1976/T76	19 (dlvd.)	55.6	I, II
75354	1,1-Dichloroethylene	170x10^6 lbs./1975/SRI	--	--	I, II
57749	1,2,4,5,6,7,8,8-Octachlor-2,3,3a,4,7,7a-hexahydro-4,7-methanoindane (chlordane)	21x10^6 lbs./1974/SRI (consumption)	105 (frt.alld.)	22	I, II
116143	Tetrafluoroethylene	17.3x10^6 lbs./1975/T75	--	--	--
76448	1,4,5,6,7,8,8-Heptachloro-3a,4,7,7,7a-tetrahydro-4,7-methanoindane (heptachlor)	2x10^6 lbs./1974/SRI (consumption)	175 (frt.alld.)	3.5	I, II

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*Taken from Chemical Marketing Reporter, April 25, 1977, reflecting the list prices prevailing for large lots.

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Unsaturated Hydrocarbons

HALOGENATED UNSATURATED HYDROCARBONS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
75025	Fluoroethylene (Vinyl fluoride)	>1000 lbs./1975/T75
75387	1,1-Difluoroethylene (Vinylidene fluoride)	>1000 lbs./1975/T75
78886	2,3-Dichloropropene	>1000 lbs./1975/T75
79356	1,1-Dichloro-2-2-difluoroethylene	>1000 lbs./1976/SRI
79389	Chlorotrifluoroethylene	>1000 lbs./1975/T75
96195	1,2,3-Trichloropropene	>1000 lbs./1975/T75
106956	3-Bromopropene	>1000 lbs./1976/SRI
107051	3-Chloropropene	>1000 lbs./1975/T75
116154	Hexafluoropropene	>1000 lbs./1975/T75
542756	1,3-Dichloropropene	>1000 lbs./1975/T75
563473	3-Chloro-2-methyl-1-propene	>1000 lbs./1975/T75
593602	Bromoethene (Vinyl bromide)	>1000 lbs./1975/T75
760236	3,4-Dichlorobutene-1	>1000 lbs./1976/SRI
764410	1,4-Dichloro-2-butene	>1000 lbs./1975/T75
1653196	2,3-Dichloro-1,3-butadiene	>1000 lbs./1975/T75
--	1-Chloro-3-methyl-3-butene	>1000 lbs./1975/T75
--	Pentachloropropene	>1000 lbs./1975/T75

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Unsaturated Hydrocarbons

HALOGENATED UNSATURATED HYDROCARBONS WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
360894	Perfluorobutene-2
513315	2,3-Dibromopropylene
593613	Acetylene bromide
--	Chloropentafluoropentene

b. Class IVB: Halogenated Methanes

There are eight members of this class with an annual U.S. production greater than one million pounds. However, one of these, methyl bromide, is used almost exclusively as a pesticide and will not be discussed further.

Three of the chemicals are fluorocarbons which have been reviewed in great depth in two reports prepared in 1975: "Economic Significance of Fluorocarbons," Office of Business Research and Analysis, Bureau of Domestic Commerce, U.S. Department of Commerce (December 1975) and "Preliminary Economic Impact Assessment of Possible Regulatory Action to Control Atmospheric Emissions of Selected Hydrocarbons" (PB 247115). These two reports cover so many facets of the subject that SRI felt that it would be inappropriate to try to prepare a condensed version for this report. The information regarding uses of the fully halogenated fluorocarbons was recently brought up to date as part of the notice of proposed rulemaking which the EPA published in the Federal Register on May 13, 1977 (pp. 24542-24549). In view of the availability of these documents, it was felt that the time and funds which would be required to prepare a market forecast on the fluorocarbons would be better spent on other parts of this research request.

Because the other four chemicals have different use patterns, they will be discussed individually.

Carbon tetrachloride

U.S. production of carbon tetrachloride in recent years has been as follows (millions of pounds): 1974 (1,163); 1975 (907); and 1976 (850). U.S. imports of carbon tetrachloride were 16.4 million pounds in 1975 and 7.0 million pounds in 1976. U.S. exports totaled 27.2 million pounds in 1975 and 15.7 million pounds in 1976.

The estimated U.S. domestic consumption pattern for carbon tetrachloride in 1975 was: 58% as an intermediate for production of dichlorodifluoromethane; 35% as an intermediate for production of trichlorofluoromethane; and 7% for miscellaneous applications (includes exports, solvent uses, grain fumigation, pesticides, and formulation of gasoline additives).

With 93% of carbon tetrachloride consumption accounted for in the production of two fluorocarbons, its future production levels are dependent on the markets for these chemicals. These two fluorocarbons have traditionally been the two largest volume fluorocarbons and have found widespread use as aerosol propellants and as refrigerants. In recent years, they have been under investigation because of concern about their potential effect on the ozone level of the stratosphere. As a consequence, several government agencies have taken steps to reduce or ban their use in aerosols and restrictions on their use as refrigerants are under study.

U.S. consumption of carbon tetrachloride as a fumigant (principally for grain) is estimated to have been about 20 million pounds in 1975. The continued use as a fumigant is in doubt since the EPA has included carbon tetrachloride in a list of pesticides which are candidates for an RPAR action. A notice of such action is required by October 1, 1977. If the action is taken, the final outcome could be limitations or banning of carbon tetrachloride as a pesticide.

In the light of all of these developments, annual U.S. production of carbon tetrachloride is expected to continue the declines shown in 1975 and 1976.

Methylene chloride

U.S. production of this chemical (which is also known as dichloromethane) in recent years has been as follows (millions of pounds): 1974 (609);

1975 (497); and 1976 (537). U.S. imports were only 12 million pounds in 1974 and 1975 but increased to 42 million pounds in 1976. U.S. exports totaled 97 million pounds in 1975.

The estimated U.S. domestic consumption pattern for methylene chloride in 1974 was: 43% as an ingredient of paint removers, 24% in solvent degreasing, 12% in plastics processing, and 21% as an aerosol vapor pressure depressant and in other miscellaneous applications (e.g., mostly solvent applications in the pharmaceutical, food, photography, and fiber industries).

In early 1977, the consumption of methylene chloride was expected to increase at an average annual rate of 9% for the period 1974-1985. This projection was based largely on its potential use as an aerosol component and as a blowing agent for polyurethane foams, markets which have been dominated by fluorocarbons in the past. Methylene chloride is said to reduce flammability of aerosols, help dissolve resins, and prevent valve clogging. Its future growth in this market will probably depend to a considerable degree on whether the present indications that it is not a threat to the ozone layer and that it is not a carcinogen are substantiated by further tests.

Methylene chloride is used in industrial paint removers where it offers an advantage over alkaline products because it does not attack aluminum. In household paint remover formulations, nonflammability and low toxicity have helped it to dominate this market. Although it has a low boiling point and good stability which make it of interest for some metal cleaning operations, apparently it is not expected to compete successfully with methyl chloroform (1,1,1-trichloroethane) for the bulk of this market.

Methyl chloride

U.S. production of methyl chloride in recent years has been reported as follows (millions of pounds): 1974 (493); 1975 (367); and 1976 (372).

These figures may be understatements of total production because some methyl chloride is produced but not separated or measured and therefore not reported by some producers. Data on U.S. imports and exports of methyl chloride are not available.

Nearly all current U.S. production of methyl chloride is based on the reaction of hydrogen chloride with methanol. In several plants, the methyl chloride may not be isolated before treatment with chlorine to produce methylene chloride, chloroform, or carbon tetrachloride. Excluding the methyl chloride used in this manner, the estimated U.S. consumption pattern in 1974 was: 50% as an intermediate for production of silicones, 30% as a tetramethyl lead intermediate, 5% as a catalyst solvent in butyl rubber manufacture, and 15% for miscellaneous uses (e.g., production of methyl cellulose, N-methyl quaternary ammonium compounds, methyl mercaptan, and pesticides).

In 1976, future growth in methyl chloride demand was estimated at 6% annually through 1980 by one source. Any growth will largely depend on the consumption of silicones and tetramethyl lead. New markets for silicones as PCB replacements in electrical transformer, in brake fluids, and as elastomers are developing which should increase methyl chloride consumption but continuation of the decline in U.S. consumption of lead alkyls (see discussion under Ethyl chloride) will have the reverse effect. Concern about the toxic properties of the methanearsonate herbicides derived from methyl chloride has prompted the EPA to put these chemicals on a list of candidates for RPAR action. Such action could lead to restrictions of their usage and reduce this market for methyl chloride (which is estimated to have consumed 12 million pounds of methyl chloride in 1974).

Other methylating agents could be used to replace methyl chloride in most of its applications but the potential substitutes (e.g., dimethyl sulfate, methyl bromide, methyl iodide) are much more expensive and have toxicity and handling problems which make them less desirable.

The silicones industry is based largely on the use of the various methyl chloride-derived methyl chlorosilanes as intermediates. Although chlorosilanes having other substituents are produced commercially, it is not known whether they can be used to produce polymers with the desired properties. The alternatives to lead alkyls such as tetramethyl lead are discussed above.

Chloroform

U.S. production of this chemical in recent years has been as follows (millions of pounds): 1974 (302); 1975 (262); and 1976 (291). U.S. imports of chloroform were 1.5 million pounds in 1974 and 5.6 million pounds in 1975. U.S. exports totaled 12.0 million pounds in 1975 and 19.4 million pounds in 1976.

The estimated U.S. domestic consumption pattern for chloroform in 1974 was: 75% as an intermediate for the production of chlorodifluoromethane; and 25% in miscellaneous applications (e.g., in antibiotics purification and other solvent uses, as an intermediate in the preparation of other chemicals, and as an ingredient in fumigants).

The level of future production of chloroform will depend largely on the market performance of chlorodifluoromethane (Fluorocarbon 22). This chemical (which has been used largely as a refrigerant, as a blowing agent for plastics, and as a chemical intermediate for the production of tetrafluoroethylene) was being developed for use in consumer aerosols until late 1976 when tests indicated that it might be mutagenic. The EPA is reported to be considering regulations to restrict emissions of fluorocarbons from refrigerants in the future.

Three other recent developments with impact on other uses of chloroform are that: (1) an RPAR action on the use of chloroform in pesticides was taken in April 1976 but no final decision on registration has yet been reached; (2) effective July 29, 1976, the FDA banned the use of chloroform in drug or cosmetics products; and (3) in May 1977, OSHA announced that it would take appropriate action on a petition to lower the standard for occupational exposure.

As discussed under Tetrafluoroethylene, consumption of this monomer for fluorocarbon resins is expected to increase in the future and this will require larger amounts of chlorodifluoromethane for the synthesis.

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Methanes

HALOGENATED METHANES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
56235	Carbon tetrachloride	907x10^6 lbs./1975/T75	14.5 (frt. alld.)	132	I, II
75092	Methylene chloride (Dichloromethane)	497x10^6 lbs./1975/T75	16 (T75)	79.5	I, II
75718	Dichlorodifluoromethane	393x10^6 lbs./1975/T75	41 (T75)	161	I, II
74873	Methyl chloride (Chloromethane)	366x10^6 lbs./1975/T75	15 (works)	54.9	--
75694	Trichlorofluoromethane	270x10^6 lbs./1975/T75	34 (T75)	91.8	I
67663	Chloroform	262x10^6 lbs./1975/T75	20 (delivered)	52.4	I, II
75456	Chlorodifluoromethane	132x10^6 lbs./1975/T75	79 (T75)	104	I
74839	Methyl bromide (Bromomethane)	36.0x10^6 lbs./1975/SRI	41 (frt. alld.)	14.8	--

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*Taken from Chemical Marketing Reporter, April 25, 1977, reflecting the list prices prevailing for large lots. Values designated as coming from Synthetic Organic Chemicals, United States Production and Sales (T75), are unit sales value which is calculated from total quantities sold (the sum of the large quantities sold on a contractual basis and smaller quantities sold intermittently) and total sales value (the sum of the values of sales at contract prices and list prices).

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Methanes

HALOGENATED METHANES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
74884	Methyl iodide (Iodomethane)	18.9×10^3 lbs./1973/T73
74953	Dibromomethane (Methylene bromide)	2.2×10^3 lbs./1975/SRI
74975	Bromochloromethane	>1000 lbs./1975/T75
75116	Diiodomethane (Methylene iodide)	>1000 lbs./1975/T75
75274	Bromodichloromethane	>1000 lbs./1976/SRI
75434	Dichlorofluoromethane	>1000 lbs./1975/T75
75467	Trifluoromethane	>1000 lbs./1975/T75
75478	Iodoform	>1000 lbs./1976/SRI
75616	Dibromodifluoromethane	>1000 lbs./1976/SRI
75627	Bromotrichloromethane	>1000 lbs./1975/T75
75638	Bromotrifluoromethane	>1000 lbs./1975/T75
75729	Chlorotrifluoromethane	>1000 lbs./1975/T75
75730	Tetrafluoromethane	>1000 lbs./1975/T75
558134	Tetrabromomethane (Carbon tetrabromide)	>1000 lbs./1976/SRI
--	Chlorofluoromethane	>1000 lbs./1976/SRI

Revised 8/77

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Methanes

HALOGENATED METHANES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
75252	Tribromomethane
--	Bromotrifluoromethane
--	Carbon tetraiodide
--	Dichloroiodomethane
--	Difluoromethane

c. Class IVC: Halogenated Aryl Derivatives

Twenty-seven members of this class have an annual U.S. production greater than one million pounds. However, twenty-one of these chemicals are used almost exclusively as pesticides and will not be discussed further. Because the six remaining chemicals have different use patterns, they will be discussed individually.

Monochlorobenzene

U.S. production of monochlorobenzene (also known as chlorobenzene) in recent years has been as follows (millions of pounds): 1974--379; 1975--306; and 1976--329. U.S. imports through principal U.S. customs districts totaled 1.49 million pounds in 1974 and 8.37 million pounds (principally from Poland) in 1975. Data on U.S. exports of monochlorobenzene are not available.

The U.S. consumption pattern for monochlorobenzene in 1974 was: solvent applications (e.g., for pesticides; in degreasing operations), 49%; intermediate for chloronitrobenzenes (dye and pesticide intermediates), 30%; intermediate for diphenyl oxide, 8%; intermediate for DDT, 7%; and other uses, 6%. Consumption of monochlorobenzene is expected to grow at an average annual rate of 1-2%, provided governmental regulations do not significantly restrict its use as a solvent for pesticides.

In the absence of information on the specific solvent uses of monochlorobenzene, the availability of substitutes for this use cannot be determined. In the uses as an intermediate, substitutes are generally not available, but substitutes are available in some cases for the end products. Thus, the nitrochlorobenzenes are used to make nitrophenols, which in turn are used to make phosphate and carbamate insecticides for which there are substitutes. U.S. production of DDT is essentially all exported for public health uses, an application where DDT appears to be the preferred agent in spite of concern over its environmental effects.

alpha-Chlorotoluene

U.S. production of alpha-chlorotoluene (more commonly known as benzyl chloride) in recent years is estimated to have been as follows (millions of pounds): 1974--99; 1975--70; and 1976--90. Data on U.S. imports and exports are not available but imports and exports are believed to be minor.

The U.S. consumption pattern for alpha-chlorotoluene in 1975 is estimated to have been as follows: intermediate for n-butyl benzyl phthalate, 67%; intermediate for benzyl alcohol, 13%; intermediate for quaternary ammonium compounds, 12%; intermediate for benzyl acetate, 2%; and other applications, 6%.

U.S. consumption of alpha-chlorotoluene is expected to grow at an average annual rate of 5-7% through 1980.

n-Butyl benzyl phthalate is a polyvinyl chloride plasticizer primarily used in vinyl flooring. U.S. production is expected to grow 5-6% per year over the next few years. n-Butyl benzyl phthalate is often used in conjunction with di(2-ethylhexyl)phthalate, the most widely used general polyvinyl chloride plasticizer, and di(2-ethylhexyl)phthalate is probably a likely substitute for it.

Benzyl alcohol, which can also be produced by the catalytic reduction of benzaldehyde, is chiefly used as a textile dye assistant for nylon and wool. It is also used for the manufacture of esters, photographic chemicals, perfumes, cosmetics, and pharmaceuticals. Because demand for benzyl alcohol is declining in the textile industry, alpha-chlorotoluene consumption for its manufacture may have dropped dramatically by 1980.

alpha-Chlorotoluene is used to manufacture quaternary ammonium compounds (e.g., dodecyldimethyl benzyl quaternary ammonium chloride) which are used as germicides, to sanitize food processing equipment, and as algicides in residential swimming pools. Small amounts are used as hair conditioners, dispersing agents, preservatives for emulsion paints, emulsifying and demulsifying agents, wetting agents, in room deodorizers, and in the production of surface-modified clays.

Benzyl acetate, which can also be manufactured from benzyl alcohol, is used in perfumes and as a high boiling solvent for resins, oils, lacquers, polishes, and inks.

Other applications for alpha-chlorotoluene include its use in the manufacture of a variety of esters (used in the pharmaceutical, flavor, and perfume industries); benzylamine (used as a dye and pharmaceutical intermediate); benzyldimethylamine (a dehydrogenation catalyst); and as a dye intermediate for triphenylmethane dyes.

ortho-Dichlorobenzene

U.S. production of o-dichlorobenzene in 1975 was 54.7 million pounds, and 1976 production is estimated to have been 85 million pounds. Reported production of dichlorobenzenes was understated in 1975 because all producers did not report to the U.S. International Trade Commission. U.S. imports of o-dichlorobenzene through principal U.S. customs districts totaled 1.63 million pounds in 1974 and 110 thousand pounds in 1975 (when a reported 2.6 million pounds of "o-dichlorobenzene, mixed" was also imported). Combined U.S. exports of all dichlorobenzenes amounted to 981 thousand pounds in 1975 and 2.58 million pounds in 1976.

The estimated U.S. consumption pattern for o-dichlorobenzene in 1975 was: 65% in organic synthesis (mainly for 3,4-dichloroaniline); 15% as a toluene diisocyanate process solvent, 10% for miscellaneous solvent usage (e.g., paint removers, engine cleaners, and de-inking solvents), 5% in dye manufacture, and 5% for miscellaneous uses.

Future growth in production of o-dichlorobenzene will depend principally on the markets for the organic chemicals which are manufactured from it. The single most important derivative is believed to be 3,4-dichloroaniline, which is a key intermediate in the manufacture of the amide herbicide, propanil (3',4'-dichloropropionanilide), and the two urea herbicides, diuron (3-[3,4-dichlorophenyl]-1,1-dimethylurea), and neburon (1-n-butyl-3-[3,4-dichlorophenyl]-1-methylurea). Propanil is the most important of these, with an estimated 1975 U.S. consumption of 9 million pounds. It is all used on rice and represents over 70% of the total U.S. rice herbicide market (where it competes mainly with a thiocarbamate herbicide, molinate). Estimated 1975 U.S. consumption of diuron was 4.5 million pounds (mostly in non-agricultural uses) and 1975 consumption of neburon is believed to have been less than 100 thousand pounds.

Monochlorobenzene is also presently being used as a solvent in the toluene diisocyanate process. High prices for benzene and chlorine have made o-dichlorobenzene an expensive solvent and cheaper substitutes may start to replace it in this end use market

o-Dichlorobenzene is used to manufacture three dyes; C.I. Mordant Red 27, C.I. Direct Blue 108, and C.I. Direct Violet 54. C.I. Direct Blue 108 is also presently produced by a methods not using o-dichlorobenzene. C.I. Direct Violet 54 is also produced by a method using nitrobenzene in place of o-dichlorobenzene. No substitute is presently known for o-dichlorobenzene in the manufacture of C.I. Mordant Red 27.

para-Dichlorobenzene

U.S. production of p-dichlorobenzene was 45.8 million pounds in 1975, and 1976 production is estimated to have been 70 million pounds. Reported production of dichlorobenzenes was understated in 1975 because all producers did not report to the U.S. International Trade Commission. Data on U.S. imports of p-dichlorobenzene are not available. Combined U.S. exports of all dichlorobenzenes amounted to 981 thousand pounds in 1975 and 2.58 million pounds in 1976.

The estimated U.S. consumption pattern for p-dichlorobenzene in 1975 was: 50% as a space odorant; 40% for moth control; and 10% for miscellaneous uses.

Future growth in p-dichlorobenzene demand through 1980 is expected to be minimal. As a space odorant, p-dichlorobenzene is used to mask odors in toilets and in garbage and refuse containers. o-Dichlorobenzene can be used as a substitute for p-dichlorobenzene in this end use. Although refined naphthalene has been widely used for moth control, increased acceptance of p-dichlorobenzene has resulted in a decline in the demand for naphthalene for this end use. The substitution of synthetic fibers for wool has resulted in a general decline in demand for all moth control agents in recent years, and this will probably continue.

N-Acetylsulfanilyl chloride

U.S. production of N-acetylsulfanilyl chloride was 5.6 million pounds in 1974 and 4.1 million pounds in 1975. No sales were reported to the U.S. International Trade Commission by the manufacturers, indicating that this chemical is used captively as an intermediate for the production of other chemicals. U.S. imports through the principal U.S. customs districts were 2 thousand pounds in 1974 and 529 thousand pounds in 1975. Data on U.S. exports are not available.

The only known use for N-acetylsulfanilyl chloride is as an intermediate in the production of sulfa drugs such as sulfadiazine, sulfathiazole, sulfanilamide, and sulfamethazine. Annual production of the sulfa drugs averaged 6 million pounds during 1971-1975, with extremes of 7.1 million pounds in 1974 and 4.7 million pounds in 1975. No significant change in the future level of production of sulfa drugs is indicated. Other N-acylsulfanilyl chlorides can be substituted for the N-acetyl intermediate. Also, p-Nitrobenzenesulfonyl chloride can be used instead of the N-acylsulfanilyl chlorides, followed by reduction of the nitro group to give the respective sulfa drugs. Either of these alternate methods of production would be more costly than the current process using N-acetylsulfanilyl chloride.

(Mixed alkyl)phenoxypoly(ethyleneoxy)ethyl chloride

Data on U.S. production of this chemical are not reported because it is manufactured commercially by only one U.S. company. Data on U.S. imports and exports are also not available.

U.S. annual production is estimated to greater than 1 million pounds primarily on the basis that this chemical is believed to be an important ingredient in some of the major brands of household automatic dishwasher detergents. The structure of this chemical is identical with that of the major nonionic surfactants, the ethoxylated (mixed alkyl)phenols, except that the hydroxyl group at the end of the polyoxyethylene chain has been replaced by chlorine. This one difference is the basis for the use of this chemical in the dishwasher detergent application. It retains much of the surface-active properties of the ethoxylated alkyl phenols, but creates far less foam--a property which is extremely desirable in a dishwasher detergent. It is believed that two other related compounds, (mixed alkyl)phenol, butyl ether, and nonylphenoxypoly(ethyleneoxy)ethyl iodide, plus a fatty alcohol derivative, decyloxypoly(ethyleneoxy)ethyl chloride, are also used in dishwasher detergents for the same purpose but this could not be verified.

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Aryl Derivatives

HALOGENATED ARYL DERIVATIVES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
NF 108907	Monochlorobenzene	$306x10^6$ lbs./1975/T75	26 (frt.alld.)	80	I
100447	alpha-Chlorotoluene (Benzyl chloride)	$90x10^6$ lbs./1976/SRI	37 (frt.alld.)	33	I,II
15972608	2-Chloro-2',6'-diethyl-N-(methoxymethyl)-acetanilide (alachlor)	$81x10^6$ lbs./1975/SRI (consumption)	p*	--	--
94757	2,4-Dichlorophenoxyacetic acid (2,4-D)	$59x10^6$ lbs./1974/SRI	83 (works, frt. equald.)	49	--
NF 95501	o-Dichlorobenzene	$55x10^6$ lbs./1975/T75	31 (frt.alld.)	17	I
NF 106467	p-Dichlorobenzene	$46x10^6$ lbs./1975/T75	22 (works)	10	I
87865	Pentachlorophenol (PCP)	$39x10^6$ lbs./1975/T75	42 (frt.alld.)	16	--
1918167	2-Chloro-N-isopropylacetanilide (Propachlor)	$11x10^6$ lbs./1975/SRI (consumption)	p	--	--
133904	2,5-Dichloro-3-aminobenzoic acid, ammonium salt (amiben)	$10x10^6$ lbs./1975/SRI (consumption)	p	--	IA
93765	2,4,5-Trichlorophenoxyacetic acid (2,4,5-T)	$6.7x10^6$ lbs./1975/SRI (consumption)	112 (works)	7.5	--
330552	3-(3,4-Dichlorophenyl)-1-methoxy-1-methylurea (linuron, Lorox®)	$5.4x10^6$ lbs./1975/SRI (consumption)	p	--	--

HALOGENATED ARYL DERIVATIVES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
1861321	Dimethyl-2,3,5,6-tetrachloroterephthalate (DCPA, Dacthal®)	4.6×10^{6} lbs./1975/SRI (consumption)	p	--	--
330541	3-(3,4-Dichlorophenyl)-1-1-dimethyl urea (diuron)	4.5×10^{6} lbs./1975/SRI (consumption)	p	--	--
121608	N-Acetylsulfanilyl chloride	4.1×10^{6} lbs./1975/T75	--	--	--
94746	4-Chloro-2-methylphenoxyacetic acid (MCPA)	3.9×10^{6} lbs./1975/SRI (consumption)	p	--	--
1897456	2,4,5,6-Tetrachloroisophthalonitrile (Chlorothalonil)	3.5×10^{6} lbs./1975/SRI (consumption)	p	--	IA
1918009	3,6-Dichloro-2-anisic acid (dicamba, Banvel®)	2.8×10^{6} lbs./1975/SRI (consumption)	p	--	--
82688	Pentachloronitrobenzene (PCNB, Terraclor®)	2.3×10^{6} lbs./1975/SRI (consumption)	p	--	IA, I, II
93721	2-(2,4,5-Trichlorophenoxy) propionic acid (plus esters and salts) (Silvex)	2×10^{6} lbs./1975/SRI (consumption)	p	--	I, II
133073	N-Trichloromethylthiophthalimide (Folpet, Phaltan®)	1.8×10^{6} lbs./1975/SRI (consumption)	p	--	--

HALOGENATED ARYL DERIVATIVES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
6164983	N'-(4-Chloro-o-tolyl)-N,N-dimethyl-formanidine (chlordimeform)	1.3x10^6 lbs./1974/SRI (consumption)	p	--	I, II
786196	5-((p-Chlorophenylthio)methyl) 0,0-diethyl phosphorodithioate (carbophenothion)	1.2x10^6 lbs./1974/SRI (consumption)	p	--	--
101213	Isopropyl m-chlorocarbanilate (Chlorpropham)	1.1x10^6 lbs./1974/SRI (consumption)	p	--	--
299843	Dimethyl 2,4,5-trichlorophenyl phosphorothionate (Ronnel)	1.1x10^6 lbs./1974/SRI (consumption)	p	--	--
299865	4-tert-Butyl-2-chlorophenyl-O-methyl methyl phosphoroamidate (Crufomate)	1x10^6 lbs./1974/SRI (consumption)	p	--	--
13360457	3-(4-Bromo-3-chlorophenyl)-1-methoxy-1-methylurea (chlorbromuron)	1x10^6 lbs./1975/SRI (consumption)	p	--	--
--	(Mixed alkyl)phenoxypoly(ethyleneoxy) ethyl chloride	>1x10^6 lbs./1976/SRI	--	--	--

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[*] Taken from Chemical Marketing Reporter, April 25, 1977, reflecting the list prices prevailing for large lots. Since many of these chemicals (indicated by p in price column) find use only as pesticides, no additional effort was made to obtain prices for them.

NF Indicates halogenated aryl compounds having no other functional groups.

Revised 8/77

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Aryl Derivatives

HALOGENATED ARYL DERIVATIVES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
23950585	N-(1,1-Dimethylpropynyl)-3,5-dichlorobenzamide (Kerb®)	800×10^3 lbs./1975/SRI (consumption)
2310170	O,O-Diethyl S-((6-chloro-2-oxobenzoxazolin-3-yl)-methyl)phosphorodithioate (phosalone)	600×10^3 lbs./1974/SRI (consumption)
99309	2,6-Dichloro-4-nitroaniline	500×10^3 lbs./1974/SRI (consumption)
1689845	3,5-Dibromo-4-hydroxybenzonitrile (bromoxynil)	500×10^3 lbs./1974/SRI (consumption)
101279	2-Butynyl-4-chloro-m-chlorocarbanilate (Carbyne®)	400×10^3 lbs./1975/SRI (consumption)
120365	2-(2,4-Dichlorophenoxy)propionic acid (2,4-DP)	400×10^3 lbs./1975/SRI (consumption)
150685	3-(p-Chlorophenyl)-1,1-dimethylurea (monuron)	200×10^3 lbs./1975/SRI (consumption)
1194656	2,6-Dichlorobenzonitrile	200×10^3 lbs./1975/SRI (consumption)
--	2,5-Diethoxy-4-morpholinobenzenediazonium chloride	170×10^3 lbs./1975/T75
97096	4-Chloro-3-nitrobenzenesulfonamide	170×10^3 lbs./1975/T75
--	p-Diethylaminobenzenediazonium chloride	120×10^3 lbs./1975/T75
2675776	1,4-Dichloro-2,5-dimethoxybenzene (chloroneb)	100×10^3 lbs./1975/SRI (consumption)
961115	2-Chloro-1-(2,4,5-trichlorophenyl)vinyl dimethyl-phosphate	100×10^3 lbs./1974/SRI (consumption)
94826	4-(2,4-Dichlorophenoxy)butyric acid (2,4-DB)	100×10^3 lbs./1975/SRI (consumption)

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Aryl Derivatives

HALOGENATED ARYL DERIVATIVES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
94815	4-(2-Methyl-4-chlorophenoxy)butryic acid (MCPB)	100×10^3 lbs./1975/SRI (consumption)
--	2,5-Dichloro-4-(3-methyl-5-oxo-2-pyrazolin-1-yl)-benzenesulfonic acid	50×10^3 lbs./1975/T75
827941	2,6-Dibromo-4-nitroaniline	40×10^3 lbs./1975/T75
113928	Chlorpheniramine maleate	36×10^3 lbs./1975/SRI
--	p-(Ethyl(2-hydroxyethyl)amino)benzenediazonium chloride	20×10^3 lbs./1975/T75
56757	Chloramphenicol	13×10^3 lbs./1974/SRI (sales)
NF 87821	Hexabromobenzene	>1000 lbs./1975/T75
NF 95465	o-Bromotoluene	>1000 lbs./1975/T75
104836	p,alpha-Dichlorotoluene	>1000 lbs./1975/T75
NF 106387	p-Bromotoluene	>1000 lbs./1975/T75
NF 106398	Bromochlorobenzene	>1000 lbs./1975/T75
NF 106434	p-Chlorotoluene	>1000 lbs./1975/T75
NF 108418	m-Chlorotoluene	>1000 lbs./1975/T75
NF 108861	Bromobenzene	>1000 lbs./1975/T75
NF 118741	Hexachlorobenzene	>1000 lbs./1975/T75
NF 26249127	Dibromobenzene	>1000 lbs./1975/T75

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Aryl Derivatives

HALOGENATED ARYL DERIVATIVES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
NF --	1-Bromo-2,4,6-triethylbenzene	>1000 lbs./1975/T75
--	p-Chloro-α,α,α-trifluorotoluene	>1000 lbs./1975/T75
--	Dichlorobenzyl chloride	>1000 lbs./1975/T75
NF --	2,6-Dichlorotoluene	>1000 lbs./1975/T75
--	Ethylbenzyl chloride	>1000 lbs./1975/T75
--	Nonylphenoxypoly(ethyleneoxy)ethyl iodide	>1000 lbs./1975/T75
NF --	Tetrabromo-o-chlorotoluene	>1000 lbs./1977/SRI
--	α,2,4-Trichlorotoluene	>1000 lbs./1975/T75

[NF] Indicates halogenated aryl compunds having no other functional groups.

d. Class IVD: Halogenated Polyaromatics

There are five members of this class with an annual U.S. production level of one million pounds or more. Four of these chemicals are used almost exclusively as pesticides and will not be discussed further. The remaining member of this class, the polychlorinated biphenyls (PBCs) has been reviewed in great depth by an EPA contractor and the final report of this review, "PBCs in the United States — Industrial Use and Environmental Distribution" (PB-252012), covers so many facets of the subject that preparation of a condensed version for this report was deemed inappropriate. The information regarding uses of PBCs was recently updated as part of the notice of proposed rule making which the EPA published in the Federal Register on May 24, 1977 (pp. 26564-26577). In view of the availability of these two documents, it was felt that the time and funds which would be required to prepare a market forecast on PBCs would be better spent on other parts of this research request.

Prior to 1975, hexabromobiphenyl (frequently referred to as polybrominated biphenyls or PBBs) were also produced at levels exceeding one million pounds per year. One company reportedly produced 11 million pounds of PBBs from 1970 to 1974. This chemical, a flame retardant, was accidentally fed to cattle in 1973 and found its way into the food chain. One aftereffect of this incident was that the company stopped production of PBBs in late 1974 or early 1975. The related octabromo- and decabromo-biphenyls are still produced by another company but the quantity made is believed to be much less than the amount of the hexabromobiphenyl produced in earlier years.

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Polyaromatics

HALOGENATED POLYAROMATICS WITH ANNUAL PRODUCTION

GREATER THAN ONE MILLION POUNDS

	CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
	50293	Dichlorodiphenyltrichloroethane (DDT)	$50\text{x}10^6$ lbs./1975/SRI	34 (delivered)	17	IA, I, II
NF	1336363	Polychlorinated biphenyls	$40.4\text{x}10^6$ lbs./1974/ PCB†	--	--	--
	72435	1,1,1-Trichloro-2,2-bis(p-methoxyphenyl)ethanol (Methoxychlor)	$3.4\text{x}10^6$ lbs./1974/SRI (consumption)	166	5.6	IA
	115322	4,4'-Dichloro-alpha-trichloromethylbenzhydrol (dicofol, Kelthane®)	$2.6\text{x}10^6$ lbs./1974/SRI (consumption)	p*	--	IA
	1982474	3-(p-(p-Chlorophenoxy)phenyl)-1,1-dimethylurea (chloroxuron)	$1\text{x}10^6$ lbs./1975/SRI (consumption)	p	--	--

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[*] Taken from Chemical Marketing Reporter, April 25, 1977, reflecting the list prices prevailing for large lots. Since some of these chemicals (indicated by p in price column) find use only as pesticides, no additional effort was made to obtain prices for them.

†PCBs in the United States -- Industrial Use and Environmental Distribution, U.S. Environmental Protection Agency, PB-252012 (February 25, 1976).

NF Indicates halogenated polyaryl compounds having no other functional groups.

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Polyaromatics

HALOGENATED POLYAROMATICS WITH ANNUAL PRODUCTION

GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
81492	1-Amino-2,4-dibromoanthraquinone	$857x10^3$ lbs./1974/T74
1836755	2,4-Dichlorophenyl p-nitrophenyl ether (Tok®)	$800x10^3$ lbs./1975/SRI (consumption)
--	1-Amino-2-bromo-4-hydroxyanthraquinone	$643x10^3$ lbs./1975/T75
42576023	Methyl-5-(2,4-dichlorophenoxy)-2-nitrobenzoate	$400x10^3$ lbs./1975/SRI (consumption)
--	2-Chloroanthraquinone	$254x10^3$ lbs./1971/SRI
568638	Erythrosine (F.D.&C. Red. No. 3)	$203x10^3$ lbs./1972/T72
72560	1,1-Dichloro-2,2-bis(p-ethylphenyl)ethane (88%) (Perthane®)	$200x10^3$ lbs./1974/SRI (consumption)
70304	2,2'-Methylene bis(3,4,6-trichlorophenol)	$200x10^3$ lbs./1975/SRI (consumption)
--	1-Chloroanthraquinone	$114x10^3$ lbs./1972/SRI
116290	4'-Chlorophenyl-2,4,5-trichlorophenyl sulphone (tetradifon)	$100x10^3$ lbs./1974/SRI (consumption)
2536314	Methyl-2-chloro-9-hydroxyfluorene-9-carboxylate (chloroflurenol)	$100x10^3$ lbs./1975/SRI (consumption)
81969	3-Bromo-7H-benz(DE)anthracen-7-one (3-Bromobenzanthrone)	$54x10^3$ lbs./1975/T75

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Polyaromatics

HALOGENATED POLYAROMATICS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
152750	Eosine Acid (D.&C. Red No. 21)	25×10^3 lbs./1975/T75
--	1-Chloro-2-methylanthraquinone	13×10^3 lbs./1975/T75
81287	5,14-Dichloroisoviolanthrone	>1000 lbs./1974/T74
81981	3,9-Dibromo-7H-benz(DE)anthracen-7-one	>1000 lbs./1975/T75
86522	α-Chloromethylnaphthalene, crude	>1000 lbs./1975/T75
92046	2-Chloro-4-phenylphenol	>1000 lbs./1975/T75
134838	Chloro(p-chlorophenyl)phenylmethane	>1000 lbs./1975/T75
--	5(and 8)-Amino-8(and 5)-bromo-9,10-dihydro-9,10-dioxo-1,6(and 1,7)-anthracene disulfonic acid	>1000 lbs./1975/T75
--	1-Amino-4-bromo-9,10-dihydro-9,10-dioxo-2-anthracene sulfonic acid and sodium salt	>1000 lbs./1975/T75
--	1-Amino-2-bromo-4-para-toluidinoanthraquinone	>1000 lbs./1975/T75
--	1-Amino-5-chloroanthraquinone	>1000 lbs./1975/T75
--	2-Amino-1-chloroanthraquinone	>1000 lbs./1975/T75
--	1-Amino-2-chloro-4-hydroxyanthraquinone	>1000 lbs./1975/T75

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Polyaromatics

HALOGENATED POLYAROMATICS WITH ANNUAL PRODUCTION
GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
--	1-Amino-2,4-dibromoanthraquinone	>1000 lbs./1975/T75
--	1-Amino-2,4-dichloroanthraquinone	>1000 lbs./1975/T75
--	1-Benzamido-4-bromoanthraquinone	>1000 lbs./1975/T75
--	1-Benzamido-4-chloroanthraquinone	>1000 lbs./1975/T75
--	1,4-Bis(5-chloro-1-anthraquinonylamino) anthraquinone mixture with 1,4-Bis (1-anthraquinonylamino)anthraquinone	>1000 lbs./1975/T75
--	1-Bromo-4-(methylamino)anthraquinone	>1000 lbs./1974/T74
NF --	1-Bromonaphthalene	>1000 lbs./1975/T75
-	Chlorobenzathrone	>1000 lbs./1975/T75
NF --	Chloronaphthalenes	>1000 lbs./1975/T75
--	1-Chloro-5-nitroanthraquinone	>1000 lbs./1975/T75
--	4-Chloro-alpha-phenyl-ortho-cresol	>1000 lbs./1975/T75
NF --	Decabromobiphenyl or ether	>1000 lbs./1977/SRI*
--	1,4-Diamino-2,3-dichloroanthraquinone	>1000 lbs./1975/T75

Class: Halogenated Hydrocarbons and Derivatives, Halogenated Polyaromatics

HALOGENATED POLYAROMATICS WITH ANNUAL PRODUCTION
GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
--	1,5-Dichloroanthraquinone	>1000 lbs./1974/T74
--	1,5(and 1,8)-Dichloroanthraquinone	>1000 lbs./1974/T74
--	Dichlorobenzanthrone	>1000 lbs./1975/T75
NF --	Octabromobiphenyl	>1000 lbs./1977/SRI*
--	1,4,5,8-Tetrachloroanthraquinone	>1000 lbs./1974/T74

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*One company produced approximately 100,000 pounds of decabromobiphenyl and octabromobiphenyl in 1970-1973.

NF Indicates halogenated polyaryl compounds having no other functional groups.

Revised 8/77

Class: Halogenated Hydrocarbons and Derivatives

HALOGENATED POLYAROMATICS WITH ANNUAL PRODUCTION

LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
81345	5,13-Dibromo-8,16-pyranthrenedione
NF 36355018	Hexabromobiphenyl

NF Indicates halogenated polyaryl compounds having no other functional groups.

5. Class V: Hydrazines, Hydroxylamines, and Carbamates

a. Class VA: Hydrazines

Of the six chemicals in this class that have an annual production greater than one million pounds, three -- maleic hydrazide, metribuzin, and Amitrole -- find use only as pesticides and will not be discussed further.

Hydrazine and Hydrazine Hydrate

These chemicals will be discussed together, since commercial production of hydrazine results in the hydrated form which then is distilled if anhydrous hydrazine is desired. The combined production of hydrazine and hydrazine hydrate has been estimated to have been 37 million pounds in 1974. Separate U.S. imports and exports data for these compounds are not available.

Approximately 60% (22 million pounds) of the 1974 production was consumed in the anhydrous form as a storable liquid rocket fuel. Of the remaining 40% (15 million pounds), approximately 10.4 million pounds (28% of total consumption) were used as a corrosion inhibitor (where it functions as an oxygen scavenger) for boiler water treatment for power utilities, pulp and paper mills, textile mills, and chemical processing plants, and as a chemical intermediate in the production of chemical blowing agents (e.g., 2,2'-azobis(isobutyronitrile), benzenesulfonic acid hydrazide (Porofor BSH), and p,p'-oxybis(benzenesulfonhydrazide)) used in the production of foamed plastics, especially polyvinyl chloride. Approximately 1.1 million pounds (3% of total consumption) were used in the manufacture of herbicides (e.g., maleic hydrazide and metribuzin) and the remaining

3.3 million pounds (9% of total consumption) were consumed in a number of applications including as an intermediate in the manufacture of pharmaceuticals (e.g., isoniazid and hydralazine), as a chemical agent for chromium reduction in process wastes, and as a corrosion inhibitor in the petroleum industries. The demand for hydrazine for both the U.S. and world markets is expected to increase 15 to 17% a year (average for all uses) until 1985.

Possible substitutes for hydrazine rocket fuels include RP-1 (a hydrocarbon fuel with a hydrogen/carbon ration of 2.0), liquid oxygen and liquid hydrogen (these are not storable), and solid rocket fuels (used in small ballistic missiles). However, hydrazine combines storability with high specific impulse, so a direct substitute without loss of performance for some military applications is not presently available.

Sodium sulfite is also used in boiler water to control corrosion but a soluble salt results from its reaction with oxygen, necessitating more frequent blowdowns to avoid exceeding permissible total dissolved solids (TDS) specifications for the boiler. Hydrazine reacts with dissolved oxygen to produce nitrogen and water, and therefore does not contribute any dissolved solids.

In its usage as a chemical intermediate in the production of pharmaceuticals, blowing agents, and herbicides, there do not appear to be any substitute chemicals for hydrazine. However, there are other blowing agents (dinitrosopentamethylenetetramine, azobisformamide, and N,N'-dimethyl-N,N'-dinitrosoterephthalamide) which could be used to replace hydrazine-derived blowing agents depending upon desired properties and application of the foamed polymer. In the pharmaceutical manufacture application, there are other non-hydrazine-derived products with similar pharmacological activity which could presumably be substituted by a competent physician. Similarly, there are other non-hydrazine-derived herbicides which probably could be substituted for metribuzin (e.g., Amiben®) and for maleic hydrazide (e.g., n-decanol).

Other chemicals presently used to reduce chromium in process wastes include SO_2, sodium sulfite, and iron filings.

Hydrazobenzene

The production of hydrazobenzene in 1975 is estimated to have been 1.2 million pounds. There were no U.S. imports or exports of hydrazobenzene reported in 1975.

In the past, hydrazobenzene was formed by the reduction of nitrobenzene during the manufacture of benzidine. However, because of the OSHA regulation covering the manufacture of benzidine, the reaction is now stopped at the hydrazobenzene step. The hydrazobenzene is then sold to dye manufacturers who convert it in closed systems to benzidine which is then further converted to one of the more than 250 benzidine-based dyes and pigments currently in use.

Possible substitute dyes for benzidine-based dyes include those produced from substituted anilines or tolidines, but the resultant products may not have as brilliant color nor be so resistant to light and washing.

Since the demand for dyes and pigments is expected to rebound from recent setbacks, demand for benzidine, and thus hydrazobenzene, is expected to increase. No information is available on which to base a quantitative forecast.

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydrazines

HYDRAZINES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
302012	Hydrazine	37×10^6 lbs./1974/SRI	160 (85%)	70	I, II
7803578	Hydrazine hydrate				
123331	Maleic hydrazide	5.8×10^6 lbs./1974/T74	254 (T74)	14.7	--
21087649	Metribuzin	3.1×10^6 lbs./1975/SRI (consumption)	--	--	--
61825	3-Amino-1,2,4-triazole (Amitrole)	1.4×10^6 lbs./1975/SRI (consumption)	--	--	IA, I, II
122667	Hydrazobenzene	1.2×10^6 lbs./1975/SRI (consumption)	--	--	--

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[*] Taken from Chemical Marketing Reporter, April 25, 1977, reflecting the list prices prevailing for large lots. Values designated as coming from Synthetic Organic Chemicals, United States Production and Sales (T74), are unit sales value which is calculated from total quantities sold (the sum of the large quantities sold on a contractual basis and smaller quantities sold intermittently) and total sales value (the sum of the values of sales at contract prices and list prices).

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydrazines

HYDRAZINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
1698608	Pyrazon (Pyramin®)	$5\text{x}10^{5}$ lbs./1975/SRI (consumption)
50339	Phenylbutazone (Butazolidin®)	<$5.5\text{x}10^{4}$ lbs./1974/SRI (sales)
129204	4-Butyl-1-(p-hydroxyphenyl)-2-phenyl-3,5-pyrazolidinedione (oxyphenbutazone)	<$2.2\text{x}10^{4}$ lbs./1974/SRI (sales)
54853	Isoniazid	>1000 lbs./1975/T75 (Stage I, II dossiers)
57147	1,1-Dimethylhydrazine (unsym-Dimethylhydrazine, UDMH)	>1000 lbs./1977/SRI (Stage I, II dossiers)
57567	Hydrazine carboxamide (semicarbazide, aminourea)	>1000 lbs./1977/SRI
57965	Sulfinpyrazone (Anturane®)	>1000 lbs./1977/SRI
59632	Isocarboxazid	>1000 lbs./1975/T75
59870	Nitrofurazone	>1000 lbs./1975/T75
59881	Phenylhydrazine hydrochloride	>1000 lbs./1975/T75
67209	Nitrofurantoin	>1000 lbs./1975/T75
67287	Nihydrazone	>1000 lbs./1977/SRI
67458	Furazolidone	>1000 lbs./1975/T75
80171	Benzenesulfonic acid hydrazide (Porofor BSH®)	>1000 lbs./1977/SRI

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydrazines

HYDRAZINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
80513	p,p'-Oxybis(benzenesulfonhydrazide)	>1000 lbs./1975/T75
80659	3-Amino-2-oxazolidinone	>1000 lbs./1977/SRI
83078	4-Aminoantipyrine (Ampyrone)	>1000 lbs./1977/SRI
86544	Hydralazine	>1000 lbs./1975/T75
98715	p-Hydrazinobenzenesulfonic acid	>1000 lbs./1975/T75
100163	(p-Nitrophenyl)hydrazine	>1000 lbs./1975/T75
103026	Acetone phenylhydrazone	>1000 lbs./1975/T75
103037	1-Carbamyl-2-phenylhydrazine (1-Phenylsemicarbazide)	>1000 lbs./1977/SRI
109273	4-Guanyl-1-nitrosoguanyl-1-tetrazine (Tetrazene)	>1000 lbs./1975/T75
109842	2-Hydrazinoethanol	>1000 lbs./1975/T75 (Stage IA dossier)
110203	Acetone semicarbazone	>1000 lbs./1975/T75
119266	2,4-Dinitrophenylhydrazine	>1000 lbs./1975/T75
142461	1,2-Hydrazinedicarbothioamide (2,5-Dithiobiurea)	>1000 lbs./1977/SRI
497187	Carbohydrazide (1,3-Diaminourea)	>1000 lbs./1977/SRI

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydrazines

HYDRAZINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
537473	4-Phenylsemicarbazide	>1000 lbs./1977/SRI
563417	Semicarbazide hydrochloride (Hydrazine carboxamide monohydrochloride)	>1000 lbs./1975/T75 (Stage IA dossier)
589219	p-Bromophenylhydrazine	>1000 lbs./1977/SRI
618406	1-Methyl-1-phenylhydrazine	>1000 lbs./1975/T75
634628	Hydrazine tartrate	>1000 lbs./1977/SRI
1156190	Tolazamide	>1000 lbs./1975/T75
1596845	Succinic acid 2,2-dimethylhydrazide (Alar®; N-Dimethylaminosuccinamic acid)	>1000 lbs./1975/T75
2644704	Hydrazine monohydrochloride	>1000 lbs./1977/SRI
5341617	Hydrazine dihydrochloride	>1000 lbs./1977/SRI
5906354	Amino hexamethyleneimine	>1000 lbs./1977/SRI
7335651	Hydrazine monoacetate	>1000 lbs./1977/SRI
7422904	Acetaldehyde 1,1-dimethylhydrazone	>1000 lbs./1977/SRI
10034932	Hydrazine sulfate (1:1)	>1000 lbs./1977/SRI
10396108	p-Toluenesulfonylsemicarbazide	>1000 lbs./1975/T75
13464807	Dihydrazine sulfate	>1000 lbs./1977/SRI

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydrazines

HYDRAZINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
13464976	Hydrazine mononitrate	>1000 lbs./1977/SRI
13775809	Hydrazine monohydrobromide	>1000 lbs./1977/SRI
14546442	Hydrazine azide	>1000 lbs./1977/SRI
20773288	Hydrazine nitroformate	>1000 lbs./1977/SRI
28860959	Carbidopa	>1000 lbs./1977/SRI
--	Aminoguanidine bicarbonate	>1000 lbs./1975/T75
--	3,5-Dinitrosalicylic acid, 5-nitrohydrazide	>1000 lbs./1975/T75
--	4-Hydrazino-m-toluenesulfonic acid	>1000 lbs./1977/SRI
--	Oxalacetic acid, diethyl ester, (p-sulfophenyl)hydrazone	>1000 lbs./1975/T75

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydrazines

HYDRAZINES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
51127	Nialamide
51718	2-Phenethylhydrazine (Phenelzine)
54922	Iproniazid
55527	Pheniprazine
60344	Methyl hydrazine
65645	(α-Methylbenzyl)hydrazine (Mebanazine)
83170	4-(Benzylideneamino)antipyrine
87150	4-Amino-2-methyl-5-pyrimidinecarboxylic acid hydrazide
114830	1-Acetyl-2-phenylhydrazine
123466	(Carboxymethyl)trimethylammonium chloride hydrazide (Girard's Reagent T)
136618	Isonicotinic acid (3-hydroxy-2,2-dimethylpropylidene)hydrazide (Pivalizid®)
140874	Cyanoacetic acid hydrazide (Cyacetacide)
284651	17,18-Dithia-3,4,11,12-tetraazatricyclo(12.2.1.16,9)octadecane
306194	Pivalic acid 2-benzylhydrazide (Pivalylbenzhydrazine)

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydrazines

HYDRAZINES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name
459869	Methylglyoxal bis(guanylhydrazone)
484231	Dihydralazine
495841	1-Isonicotinoyl-2-salicylidenehydrazine
511411	1-Acetyl-2-(3,3-diphenylhydracryloyl)hydrazine (Diphoxazide)
519653	Dioxypyramidon
530507	1,1-Diphenylhydrazine
532967	1-Benzoyl-2-phenylhydrazine
533028	Isonicotinic acid benzylidenehydrazide
536403	p-Chlorobenzhydrazide
538001	1-(m-Tolyl)semicarbazide
539640	N,N-Dimethylglycine hydrazide hydrochloride (Girard's Reagent D)
540738	1,2-Dimethylhydrazine
613945	Benzoylhydrazine
624840	Formylhydrazine
628364	1,2-Diformylhydrazine
637605	4-Methylphenylhydrazine hydrochloride (p-Tolylhydrazine hydrochloride)

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydrazines

HYDRAZINES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name
671169	N-Isopropyl-α-(2-methylhydrazino)-p-toluamide (Procarbazine)
758178	N-Methyl-N-formylhydrazine
840788	N,N'-Bis(nicotinic acid)hydrazide
840802	Isonicotinic acid m-hydroxybenzylidenehydrazide (Acroteben®)
840813	Isonicotinic acid p-hydroxybenzylidenehydrazide (Flavoteben®)
1078382	1-Acetyl-2-isonicotinoylhydrazine
1508458	Podophyllinic acid 2-ethylhydrazide
1615801	1,2-Diethylhydrazine
1741011	Trimethylhydrazine hydrochloride
1743131	Octahydro(1,2,4,5)tetrazino(1,2-a)(1,2,4,5)tetrazine
1910685	1-Methylindole-2,3-dione 3-thiosemicarbazone (Methisazone)
2757906	β-N-(γ-L(+)-Glutamyl)-4-hydroxymethylphenylhydrazine (Agaritine)
2760987	Isophthalyl dihydrazide
2779557	5,6-Dimethoxyphthaldehydic acid isonicotinoylhydrazone (Saluzid)

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydrazines

HYDRAZINES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name
3290991	p-Methoxybenzoylhydrazine
3460671	Isonicotinic acid α-methylfurfurylidenehydrazide (INF)
3530118	n-Butylhydrazine
3544352	p-(Chlorophenoxy)acetic acid 2-isopropylhydrazide (Iproclozide)
3570750	Formic acid 2-(4-(5-nitro-2-furyl)-2-thiazolyl)hydrazide
3614479	6-Hydrazino-3-pyridazinecarboxamide (Hydracarbazine)
3691745	D-Glucuronolactone isonicotinoylhydrazone
3818379	1-Methyl-2-phenoxyethyl)hydrazine (Phenoxypropazine)
3989502	N^4-Acetylsulfanilyl hydrazide
4684871	(1-Methylheptyl)hydrazine
5039612	n-Propylhydrazine
5329124	2,4,6-Trichlorophenylhydrazine
6415129	Tetramethylhydrazine
6946298	p-Aminosalicylic acid hydrazide

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydrazines

HYDRAZINES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name
6958447	Benzaldehyde 2-(2,4,6-trichlorophenyl)hydrazone
7422788	Allylhydrazine
7466548	o-Methoxybenzoylhydrazine
7654037	1-(Benzoyl)-2-(α-methylbenzyl)hydrazine (Benmoxine)
10039551	Hydrazine iodide
10309792	1-Methyl-2-benzylhydrazine
13447955	Isoniazid methanesulfonate
13482876	4-(p-Bromophenoxy)benzenesulfonohydrazide
13957363	2-Hydrazino-4,6-bis(diethylamino)-1,3,5-triazine (Hydramitrazine)
14760715	α-Hydrazinoimidazole-4(or 5)-propionic acid
16568028	Acetaldehyde N-methylformylhydrazone (Gyromitrin)
17433317	1-Acetyl-2-(α-picolinoyl)hydrazine
17749212	4-Chloro-3-(N-sulfonylhydrazino)benzoic acid
18413144	Ethylhydrazine hydrochloride

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydrazines

HYDRAZINES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name
18523698	Acetone(4-(5-nitro-2-furyl)-2-thiazolyl)hydrazone
20147255	1-Acetyl-1-ethylhydrazine
20487029	Acetaldehyde ethylhydrazone
20570961	Benzylhydrazine dihydrochloride
25939053	Benzoyl chloride (2,4,6-trichlorophenyl)hydrazone (Banamite®)
33422332	Benzoic acid 2-(2,4,6-trichlorophenyl)hydrazide
53368437	Isonicotinic acid 2-(2-acetamido-2-deoxyglucosyl)hydrazide (Inhasan)
53643519	Isonicotinic acid (1-methyl-2-morpholinoethyl)hydrazide (Tibicor)
--	N-Acetyl-N'-(4-(hydroxymethyl)phenyl)hydrazine
--	n-Amylhydrazine hydrochloride
--	4-Hydroxymethylphenylhydrazine
--	1-Methyl-2-butylhydrazine dihydrochloride
--	Pimelic acid 4-(isonicotinoyl)hydrazone

b. Class VB: Hydroxylamines*

There is only one member of this class with an annual production greater than one million pounds, hydroxylamine sulfate ($2NH_2OH \cdot H_2SO_4$). The 1975 production of hydroxylamine sulfate is estimated to be greater than 575 million pounds, most of which is produced and consumed captively in the conversion of cyclohexanone to cyclohexanone oxime (which is then converted to caprolactam). More than 99% of the caprolactam produced is used to produce nylon 6 fibers, films, and resins.

U.S. imports and exports of hydroxylamine and its salts are not available.

Hydroxylamine sulfate (and other hydroxylamine salts, including the hydrochloride, acid sulfate, nitrate, and acetate) is used in numerous non-captive applications, including: (1) as an analytical reagent in qualitative and quantitative analysis of aldehydes and ketones; (2) in treatment of acrylic fibers, polyamides, cyanoethylated cellulose, acetals of polyvinyl alcohols with cyanoaldehydes, or vinylidene cyanide, to increase the dye affinity of the polymer by forming dye-reactive sites with nitrile groups remaining in the polymer; (3) as a component of the developer solution for photographic silver emulsions; and (4) as a "short-stopping agent" to control polymer properties in emulsion polymerization of butadiene-styrene copolymers and other synthetic rubbers. No data were available on the relative amounts of hydroxylamines used in these non-captive applications.

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*includes salts and some O- and N-substituted alkyl and aryl derivatives; excludes oximes and hydroxamic acids

Since caprolactam production consumes most of the hydroxylamine sulfate, the growth rate of hydroxylamine sulfate is related to the growth rate of caprolactam consumption. The estimated average annual growth rate of caprolactam consumption for 1976-1981 is 5-6% per year. No data are available on the growth rates for the non-captive uses of hydroxylamine sulfate and other hydroxylamine salts.

There are presently two other methods used outside of the United States to produce caprolactam which use nitrosyl chloride or nitrosylsulfuric acid as intermediates rather than hydroxylamine sulfate. Depending upon the economics of the processes and licensing arrangements, these methods of producing caprolactam could presumably be used here.

Other reagents used for the qualitative and quantitative analysis of aldehydes and ketones include phenylhydrazine, 2,4-dinitrophenylhydrazine, p-bromo- or p-nitrophenylhydrazine, and semicarbazide.

Acrylic fibers and other polymers can be made more dye receptive in other ways, such as copolymerization with a monomer which is more readily dyeable or that can be converted to a dyeable derivative.

Other compounds used in the developer solution for photographic silver emulsions include hydrogen peroxide, hydrazine, pyrocatechol, hydroquinone, and 2,2',6,6'-tetramethoxy-p,p'-biphenol.

Other "shortstopping agents" used in styrene-butadiene and other synthetic rubber polymerizations include hydroquinone, sodium dimethyldithiocarbamate, and a mixture of alkylenepolyamines.

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydroxylamines

HYDROXYLAMINES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
10039540	Hydroxylamine sulfate	>575×10^6 lbs./1975/SRI	83	477	--

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*Taken from Chemical Marketing Reporter, April 25, 1977, reflecting the list prices prevailing for large lots, f.o.b. New York.

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydroxylamines

HYDROXYLAMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
135206	N-Nitroso-N-phenylhydroxylamine, ammonium salt (Cupferron)	>1000 lbs./1977/SRI
593566	O-Methylhydroxylamine hydrochloride (Methoxyamine hydrochloride)	>1000 lbs./1977/SRI
1117971	N,O-Dimethylhydroxylamine	>1000 lbs./1977/SRI
3710847	N,N-Diethylhydroxylamine	>1000 lbs./1977/SRI
4229441	N-Methylhydroxylamine hydrochloride	>1000 lbs./1977/SRI
5470111	Hydroxylamine hydrochloride	>1000 lbs./1977/SRI
10046001	Hydroxylamine acid sulfate	>1000 lbs./1977/SRI

Class: Hydrazines, Hydroxylamines, and Carbamates: Hydroxylamines

HYDROXYLAMINES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
67629	O-Methylhydroxylamine (Hydroxylamine methyl ether)
100652	N-Phenylhydroxylamine
100889	O-(Cyclohexylsulfonyl)hydroxylamine
127071	N-Carbamoylhydroxylamine (Hydroxyurea)
607307	N-1-Naphthylhydroxylamine
613478	N-2-Naphthylhydroxylamine
645885	O-(Carboxymethyl)hydroxylamine
1013203	N-1-Naphthyl-N-nitrosohydroxylamine, ammonium derivative
1121308	1-Hydroxy-2(1H)-pyridinethione (Pyrithione)
5667209	6-N-Hydroxylaminopurine
6098460	O-Benzoyl-N-methyl-N-(p-(phenylazo)phenyl)hydroxylamine
6530274	N-(p-(Phenylazo)phenyl)hydroxylamine
6810260	N-4-Biphenylylhydroxylamine
7803498	Hydroxylamine
10164337	Hydroxylamine,(ethylenedinitrilo)tetraacetate

c. Class VC: Carbamates

The chemicals in the carbamic acid esters (carbamates) class with annual production greater than one million pounds are all used only as pesticides, so no additional economic data are included beyond those summarized in the accompanying tables.

Class: Hydrazines, Hydroxylamines, and Carbamates: Carbamates

CARBAMATES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
63252	1-Naphthyl methylcarbamate (carbaryl, Sevin®)	26×10^6 lbs./1974/SRI (consumption)	250	65	I, II
1563662	2,3-Dihydro-2,2-dimethyl-7-benzofuranyl methylcarbamate (carbofuran, Furadan®)	12×10^6 lbs./1974/SRI (consumption)	735	88	--
17804352	Methyl 1-(butylcarbamoyl)-2-benzimidazole carbamate (benomyl, Benlate®)	3×10^6 lbs./1975/SRI (consumption)	1780	53	--
101213	Isopropyl m-chlorocarbanilate (chlorpropham, Furloe®)	1.1×10^6 lbs./1975/SRI (consumption)	280	3	--

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*List prices as quoted by manufacturer.

Class: Hydrazines, Hydroxylamines, and Carbamates: Carbamates

CARBAMATES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
101279	2-Butynyl-4-chloro-m-chlorocarbanilate (barban, Carbyne®)	$4x10^5$ lbs./1975/SRI (consumption) (Stage I dossier)
18413177	m-(((Dimethylamino)methylene)amino)phenyl methylcarbamate monohydrochloride (formetanate hydrochloride, Carzol®)	$4x10^5$ lbs./1974/SRI (consumption)
114261	2-Isopropoxyphenyl-N-methylcarbamate (propoxur, Baygon®)	$3x10^5$ lbs./1974/SRI (consumption, all imported)
122429	Isopropyl N-phenylcarbamate (IPC, propham)	$2x10^5$ lbs./1975/SRI (consumption)
2425061	Diethyl 4,4'-o-phenylene-bis(3-thioallophanate) (thiophanate)	$2x10^5$ lbs./1974/SRI (consumption, all imported)
23564058	Dimethyl 4,4'-o-phenylene-bis(3-thioallophanate) (thiophanate-methyl)	
2032599	4-(Dimethylamino)-m-tolyl methylcarbamate (aminocarb, Matacil®)	$1x10^5$ lbs./1974/SRI (consumption, all imported)
13684634	Methyl-m-hydroxycarbanilate m-methylcarbanilate (phenmedipham, Betanal®)	$1x10^5$ lbs./1975/SRI (consumption)
51605	(m-Hydroxyphenyl)trimethyl ammonium methyl sulfate dimethylcarbamate (Neostigmine methylsulfate)	>1000 lbs./1975/T75
51796	Ethyl carbamate	>1000 lbs./1977/SRI (Stage I and II dossiers)
57534	1,3-Propanediol, 2-methyl-2-propyl, dicarbamate (Meprobamate)	>1000 lbs./1975/T75

Class: Hydrazines, Hydroxylamines, and Carbamates: Carbamates

CARBAMATES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
78444	Carbamic acid, isopropyl-, 2-(hydroxymethyl)-2-methylpentyl ester carbamate (ester) (Carisoprodol)	>1000 lbs./1975/T75
101268	3-Hydroxy-1-methylpyridinium bromide dimethylcarbamate (Pyridostigmine bromide)	>1000 lbs./1975/T75
101655	Diphenyl 4,4'-diphenylmethylene dicarbamate	>1000 lbs./1975/T75
109580	Ethylenediamine carbamate	>1000 lbs./1975/T75
114807	(m-Hydroxyphenyl)trimethyl ammonium bromide dimethylcarbamate (Neostigmine bromide)	>1000 lbs./1975/T75
143066	Hexamethylenediamine carbamate	>1000 lbs./1977/SRI
518638	10H-Phenothiazine-10-carboxylic acid, 2-(2-(dimethylamino)ethoxy)ethyl ester, monohydrochloride (Dimethoxanate hydrochloride)	>1000 lbs./1977/SRI
532036	1,2-Propanediol, 3-(o-methoxyphenoxy)-, 1-carbamate (Methocarbamol)	>1000 lbs./1977/SRI
598550	Methyl carbamate	>1000 lbs./1975/T75
627123	n-Propyl carbamate	>1000 lbs./1977/SRI (Stage I and II dossiers)
886748	Chlorphenesin carbamate	>1000 lbs./1975/T75
1129415	m-Tolyl methylcarbamate	>1000 lbs./1975/T75

Class: Hydrazines, Hydroxylamines, and Carbamates: Carbamates

CARBAMATES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod./Year/Source
1616882	Methoxyethyl carbamate	>1000 lbs./1975/T75
2282340	3-sec-Amylphenyl-N-methylcarbamate	>1000 lbs./1975/T75
2425107	3,4-Dimethylphenyl-N-methylcarbamate	>1000 lbs./1975/T75
2631405	o-Isopropylphenyl methylcarbamate (MIPC)	>1000 lbs./1975/T75
3766812	2-sec-Butylphenyl-N-methylcarbamate (BPMC)	>1000 lbs./1975/T75 (all exported)
3942549	o-Chlorophenyl N-methylcarbamate (CPMC)	>1000 lbs./1975/T75 (all exported)
4268364	Carbamic acid, butyl-, 2-(hydroxymethyl)-2-methylpentyl ester carbamate (ester) (Tybamate)	>1000 lbs./1977/SRI
10143223	Dimethylol methoxyethyl carbamate	>1000 lbs./1974/T74
23135220	Methyl-N',N'-dimethyl-N-((methylcarbamoyl)oxy)-1-thiooxamimidate (oxamyl, Vydate®)	>1000 lbs./1975/T75
--	Bis(p-aminocyclohexyl)methane carbamate	>1000 lbs./1975/T75

Class: Hydrazines, Hydroxylamines, and Carbamates: Carbamates

CARBAMATES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
120434	1-Piperazinecarboxylic acid, ethyl ester
315184	4-Dimethylamino-3,5-xylyl methylcarbamate (mexacarbate, Zectran®) (discontinued 1974) (Stage IA dossier)
644644	2-Dimethylcarbamyl-3-methyl-5-pyrazolyl dimethylcarbamate (dimetilan)
672048	m-(1-Ethylpropyl)phenyl methylcarbamate (a component of Bux insecticide) (discontinued 1975)
70075	2-Oxazolidinone, 5-((o-methoxyphenoxy)methyl)- (Mephenoxalone)
95250	2-Benzoxazolinone, 5-chloro- (Chlorzoxazone)
533062	1,2-Propanediol, 3-(o-tolyloxy)-, 1-carbamate (Mephenesin carbamate)
1079330	4-Benzothienyl-N-methyl carbamate (Mobam®)
1665481	2-Oxazolidinone, 5-((3,5-xylyloxy)methyl)- (Metaxalone)
1746776	Isopropyl carbamate
1943799	Phenyl methylcarbamate
2032657	4-(Methylthio)-3,5-xylyl methylcarbamate (mercaptodimethur, Mesurol®)
2282340	m-(1-Methylbutyl)phenyl methylcarbamate (a component of Bux insecticide) (discontinued 1975)

CARBAMATES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name
5395017	Hydroxyethyl carbamate
16357598	1(2H)-Quinolinecarboxylic acid, 2-ethoxy-, ethyl ester (EEDQ)
22781233	2,2-Dimethyl-1,3-benzodioxol-4-yl methylcarbamate (bendiocarb, Ficam®)

6. Class VI: N-Nitroso Compounds

The only member of this class with an annual production greater than one million pounds is N-nitrosodiphenylamine. Its production in recent years has been: 1973: 2.5 million pounds (1.9 million pounds in sales); 1974: 3.5 million pounds (2.7 million pounds in sales), and 1975: 1.68 million pounds (1.1 million pounds in sales). Production was down in 1975 due to a number of factors including the recession, a long rubber workers' strike, and overstocking of rubber chemicals in 1974. Data for 1976 are not yet published, but production is expected to return to 1973 levels. U.S. imports of N-nitrosodiphenylamine were 43,000 pounds in 1973, 23,000 pounds in 1974, and none in 1975. U.S. exports of N-nitrosodiphenylamine are not published separately.

N-Nitrosodiphenylamine is used in the rubber industry as a vulcanization retarder to inhibit scorching (cross-linking) of the compounded rubber at processing temperatures, but not at vulcanizing temperatures. The use of N-nitrosodiphenylamine, as with other rubber processing chemicals, is related to the growth of rubber consumption. Industry estimates of growth in rubber consumption to 1985 vary from a low of 2.5% to a high of 5.5%.

Other compounds which have been used as vulcanization retarders by the rubber industry include salicylic acid, phthalic anhydride, and benzoic acid.

Class: N-Nitroso Compounds

N-NITROSO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Price,* ¢/lb.	Annual Prod./Year/Source	Market Value, Million $	Dossiers
86306	N-Nitrosodiphenylamine	89 (T75)	1.68x10^6 lbs./1975/T75	1.5	I

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*Unit sales value taken from *Synthetic Organic Chemicals, United States Production and Sales, 1975*, which is calculated from total quantities sold (the sum of the large quantities sold on a contractual basis and smaller quantities sold intermittently) and total sales value (the sum of the values of sales at contract prices and list prices).

Class: N-Nitroso Compounds

N-NITROSO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source	Dossiers
80115	N-Methyl-N-nitroso-p-toluenesulfonamide	>1000 lbs./1977/SRI	--
101257	3,7-Dinitroso-1,3,5,7-tetraazabicyclo(3.3.1)nonane (dinitrosopentamethylenetetramine)	>1000 lbs./1975/T75	--
133551	N,N'-Dimethyl-N,N'-dinitrosoterephthalamide	>1000 lbs./1975/T75	--
135206	N-Nitroso-N-phenylhydroxylamine ammonium salt (Cupferron)	>1000 lbs./1977/SRI	--
154938	N,N'-Bis(2-chloroethyl)-N-nitrosourea	>1000 lbs./1977/SRI	--
684935	N-Methyl-N-nitrosourea	>1000 lbs./1977/SRI	IA
18883664	Streptozotocin	>1000 lbs./1975/T75	--

Class: N-Nitroso Compounds

N-NITROSO COMPOUNDS WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
55185	Diethylnitrosamine (Stage IA dossier)
59892	4-Nitrosomorpholine
62759	Dimethylnitrosamine (Stage I and II dossiers)
70257	N-Methyl-N'-nitro-N-nitrosoguanidine
99809	N-Methyl-N,4-dinitrosoaniline
100754	1-Nitrosopiperidine
615532	N-Nitroso-N-methylurethane
621647	N-Nitroso-N-propyl-1-propaneamine (di-n-propylnitrosoamine)
759739	N-Ethyl-N-nitrosourea (Stage IA dossier)
924163	N-Butyl-N-nitroso-1-butanamine (di-n-butylnitrosoamine) (Stage IA dossier)
930552	1-Nitrosopyrrolidine
1116547	N-Nitrosodiethanolamine
4549400	N-Nitroso-N-methylvinylamine
7519360	1-Nitroso-L-proline
10595956	N-Nitrosomethylethylamine
13256229	N-Nitrososarcosine
13344508	N-Nitrososarcosine ethyl ester

Class: N-Nitroso Compounds

N-NITROSO COMPOUNDS WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name
29291358	N-Nitrosofolic acid
53759221	N-Nitrosonornicotine
--	N,N'-Dimethyl-N-nitrosourea
--	Dinitrosopiperazine
--	N-Ethyl-N-nitroso-N'-acetylurea
--	N-Methyl-N-nitroso-N'-acetylurea
--	N-Methyl-N-nitrosobiuret
--	Nitroso-sec-butyl-n-butylamine
--	Nitrosobutylphenylamine
--	Nitrosodicylcopentylamine
--	Nitrosodi-n-heptylamine
--	Nitrosodi-n-hexylamine
--	Nitrosodiisobutylamine
--	Nitrosodiisopentylamine
--	Nitrosodiisopropylamine
--	Nitrosodi-n-octylamine

Class: N-Nitroso Compounds

N-NITROSO COMPOUNDS WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name
--	Nitrosodi-n-pentylamine
--	Nitrosoethylbenzylamine
--	Nitrosoethylbutylamine
--	Nitrosoethylphenylamine
--	Nitrosoguanidine
--	Nitrosohydroxyproline
--	Nitrosomethylbutylamine
--	Nitrosomethylpropylamine
--	Nitroso-n-pentyl-n-butylamine
--	Nitroso-n-pentyl-sec-butylamine
--	Nitroso-n-pentylethylamine
--	Nitroso-n-pentylisopentylamine
--	Nitroso-n-pentylisopropylamine
--	Nitroso-n-pentyl-n-propylamine
--	Nitroso-N-phenylpiperazine
--	Nitrosopropylbutylamine

Class: N-Nitroso Compounds

N-NITROSO COMPOUNDS WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name
--	Nitroso-n-propylisopropylamine
--	N-Pentyl-N-nitrosourea
--	N,N',N'-Trimethyl-N-nitrosourea

7. Class VII: Aromatic Amines

The chemicals in this class are those with a known or estimated annual production level of one million pounds or more. Because these chemicals have use patterns which apply for the most part to the chemical rather than to the class, each chemical will be discussed individually.

3,3'-Dichlorobenzidine base and salts

Production of 3,3'-dichlorobenzidine base and salts amounted to 4.612 million pounds in 1972, the latest year in which a production figure was reported. Since only two companies reported commercial production of 3,3'-dichlorobenzidine base and salts in recent years, production figures were withheld for proprietary reasons. U.S. imports of 3,3'-dichlorobenzidine base and salts through principal U.S. customs districts amounted to 291,687 pounds in 1973 and 664,085 pounds in 1972. Imports of this chemical were not reported in 1974 and 1975. U.S. exports data for 3,3'-dichlorobenzidine base and salts are not available.

3,3'-Dichlorobenzidine base and salts are used primarily as chemical intermediates for the production of pigments. The next most important application is believed to be as a curing agent for isocyanate-containing polymers. 3,3'-Dichlorobenzidine has also had reported use in a color test for the presence of gold.

3,3'-Dichlorobenzidine base and salts are used as chemical intermediates to produce eight pigments that are produced commercially in the U.S. Five of these pigments -- C.I. Pigment Yellow 12 (1975 U.S. production - 6.028 million pounds), Pigment Yellow 14 (1.840 million pounds), Pigment Yellow 17 (415 thousand pounds), Pigment Yellow 13 (240 thousand pounds), and Pigment Yellow 55

-- are used widely in printing inks, plastics, elastomers, and in textile printing but are of secondary importance in the paint industry. Of the remaining three pigments, C.I. Pigment Orange 13 (209 thousand pounds) is used mainly to color rubber products, as well as printing inks, paper, and all types of plastics. C.I. Pigment Orange 34 (99 thousand pounds) is used in transparent metal coatings, decorative finishes, foil lacquers, tin printing, vinyl, polyethylene, and polypropylene plastics, and textile printing inks. C.I. Pigment Red 38 is used primarily in rubber, and also in plastics, inks, and paints.

There do not appear to be any substitute chemicals which could replace 3,3'-dichlorobenzidine base and salts as chemical intermediates for the production of the above-mentioned pigments. Possible chemical substitutes for these pigments can only be discussed in general terms. Besides economic considerations, choosing a specific substitute for a particular pigment depends on many physical and technical properties of the pigment that affect its usage in specific products, e.g., hue, tinctorial strength, ease of incorporation into the medium, transparency or opacity, fastness, solubility in various solvents, etc. Although many possible substitute pigments exist, the choice of these substitutes would rest with a technical pigments expert.

3,3'-Dichlorobenzidine is used alone or in blends with 4,4'-methylenebis-(2-chloroaniline) (MOCA) as a curing agent for liquid-castable polyurethane elastomers. Substitute chemicals for the use of 3,3'-dichlorobenzidine in this application include MOCA and methylenedianiline.

Since 1974, 3,3'-dichlorobenzidine (and its salts) has been listed by OSHA as a carcinogen with the result that its manufacture and use must be done in isolated systems or by closed system operations. MOCA also was listed as a carcinogen, but the standard issued in early 1974 was deleted by a court action in 1974. NIOSH has recommended that OSHA issue an Emergency Temporary Standard for MOCA, but OSHA has apparently not yet taken any further official action on MOCA. Methylenedianiline is not regulated at the present time in the workplace by OSHA.

Since the demand for pigments is expected to increase from recent setbacks, demand for 3,3'-dichlorobenzidine is also expected to increase, especially if possible OSHA legislation should eliminate the use of lead chromates pigments (annual sales of which amount to 80 million pounds). The yellow pigments derived from 3,3'-dichlorobenzidine and salts could be used as substitutes for the lead chromate pigments.

C.I. Pigment Blue 19

Production of C.I. Pigment Blue 19 during the period 1970-1972 amounted to 4.596, 3.129, and 4.484 million pounds per year, respectively. Separate production figures for C.I. Pigment Blue 19 are not available for 1973-1975; however, combined production for eight blue pigments, including C.I. Pigment Blue 19, amounted to 4.025 million pounds in 1974 and 2.267 million pounds in 1975. U.S. imports and exports data for C.I. Pigment Blue 19 are not available.

C.I. Pigment Blue 19 is used mainly in printing inks. It can also be used to color candles, in paper staining and dyeing, for copying papers and typewriter ribbons, and has had occasional use in polyvinyl chloride and rubber.

Other organic blue pigments could probably be used to replace C.I. Pigment Blue 19 in many of its applications. However, in addition to economic considerations, the choice of substitutes for C.I. Pigment Blue 19 would depend on various physical properties and performance characteristics (e.g., fastness to light and various solvents, solubility, tinctorial strength, hue, etc.) that determine the effectiveness and applicability of such pigments to their end-market uses.

4,4'-Methylenebis(N,N-dimethylaniline)

Production of 4,4'-methylenebis(N,N-dimethylaniline) amounted to 1.862 million pounds in 1974 and 1.164 million pounds in 1973. U.S. imports and exports data for this chemical are not available.

4,4'-Methylenebis(N,N-dimethylaniline) can be used as a chemical intermediate for the production of two dyes which are produced commercially in the U.S.: C.I. Basic Yellow 2 and C.I. Solvent Yellow 34. Production figures are not available for these two dyes, however. C.I. Basic Yellow 2 and C.I. Solvent Yellow 34 can also be produced from Michler's ketone, 4,4'-bis(dimethylamino) benzophenone. It is not known which chemical is more commonly used to produce these dyes.

The hydrochloride salt of this chemical is used as a reagent for lead.

No information is available on which to base any forecasts for the future growth of 4,4'-methylenebis(N,N-dimethylaniline).

N-Phenyl-2-naphthylamine

In 1975, production of N-phenyl-2-naphthylamine amounted to 1.561 million pounds, down from a production high of 4.932 million pounds in 1973. U.S. imports of N-phenyl-2-naphthylamine through principal U.S. customs districts amounted to only 167 thousand pounds in 1975. Separate U.S. exports data for this chemical are not available. It is believed that no U.S. companies are currently producing N-phenyl-2-naphthylamine commercially, due to the pending regulatory action (OSHA) that will limit the exposure of workers to it. The outlook for future production of this chemical is not promising.

N-Phenyl-2-naphthylamine has been primarily used as an antioxidant (generally at levels of 1-2%) in rubber processing to impart heat, oxidation, and flex-cracking resistance in natural rubbers, synthetic rubbers, and latexes. It has also been used as a stabilizer in electrical-insulating silicone enamels;

as an antioxidant in other polymers, in greases, and in lubricating and transformer oils; as a component of solid rocket fuels; and as a chemical intermediate for the production of the rubber antioxidant, N-phenyl-2-naphthylamine-acetone condensate.

There are many chemicals available for use as rubber antioxidants. Possible substitutes include diphenylamines, mixed diaryl-p-phenylenediamines, alkylated diphenyl-p-phenylenediamines, aldehyde-amine condensation products, ketone-amine condensation products, alkylated phenols and p-cresols, alkylated bisphenols, substituted hydroquinone, thiobisphenols, and phenol-phosphites. Selection of substitutes depends on the specific properties desired and the substrate which is treated.

C.I. Acid Blue 9

Production of C.I. Acid Blue 9* amounted to 1.37 million pounds in 1975, down from a production high of 2.136 million pounds in 1973. FD & C Blue No. 1 is chemically identical with C.I. Acid Blue 9 and differs only in purity specifications or product form. Production of FD & C Blue No. 1 amounted to 123 thousand pounds in 1975, down from 183 thousand pounds in 1973. Separate U.S. imports and exports data for these chemicals are not available.

C.I. Acid Blue 9 may be used to dye wool, silk, nylon, leather, paper, soap, and woodstains; as an indicator; and as a biological stain. It is also used as a dye in toilet bowl cleaners. Its barium salt, C.I. Pigment Blue 24, is used in printing inks, rubber, polyvinyl chloride resin, and in the production of green pigments.

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*N-ethyl-N-(4-((4-ethyl((3-sulfophenyl)methyl)amino)phenyl)(2-sulfophenyl)-methylene)-2,5-cyclohexadien-1-ylidene-3-sulfobenzenemethanaminium hydroxide inner salt disodium salt

The consumption of acid dyes, including C.I. Acid Blue 9, is expected to increase as demand for nylon carpet increases with new housing starts. Many other acid blue dyes are available, and a choice of substitutes for C.I. Acid Blue 9 would depend on various physical properties and performance characteristics (e.g., fastness, application methods, substrates, etc.) that determine the end-product usage.

FD & C Blue No. 1 is approved for use as color additive in food, drugs, and cosmetics, by the U.S. Food and Drug Administration. U.S. sales data for the first nine months of 1967 indicate that FD & C Blue No. 1 was used to color food (92%), drugs (7%), and cosmetics (1%). Based on these data, consumption of FD & C Blue No. 1 for use in food during this period was: beverages (38.3%); candy and confections (16.1%); miscellaneous foods (13.2%); bakery goods (8.9%); dessert powders (7.9%); ice cream, sherbet, and dairy products (6.3%); pet food (3.6%); cereals (2.0%); sausage (1.6%); maraschino cherries (1.4%); and snack food (0.7%).

As a drug color additive, FD & C Blue No. 1 has been used in aqueous drugs, tablets, and capsules, and its aluminum lake has found use in ointments. As a cosmetics color additive, FD & C Blue No. 1 has been used in bath salts and hair rinses, and its aluminum lake has also been used in lipsticks, rouges, face powders, and talcums.

Possible substitutes for FD & C Blue No. 1 include the only other synthetic blue food color additive approved by the FDA, FD & C Blue No. 2, and a new polymeric food dye (which is not absorbed by the bloodstream) which may be introduced to the market place by 1980.

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

	CAS No.	Chemical Name	Annual Prod. (Million Pounds)/Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
	62533	Aniline	406.93/1975/T75	23 (T75)	93.59	--
	95807	Toluene-2,4-diamine	191.01/1975/T75	90	171.91	I
	122394	Diphenylamine	39.89/1974/T74	41.1 (T75)	16.39	--
	--	N-(1,3-Dimethylbutyl)-N' -phenyl-p-phenylenediamine	30.53/1975/T75	133 (T75)	40.60	--
	1582098	α,α,α-Trifluoro-2,6-dinitro -N,n-dipropyl-p-toluidine	21.7/1975/SRI (use)	--	--	IA
	121697	N,N-Dimethylaniline	10.12/1975/T75	56 (T75)	.67	--
	133904	3-Amino-2,5-dichlorobenzoic acid, ammonium salt	10.1/1975/SRI (sales)	--	--	IA
	88744	p-Nitroaniline	8.65/1975/T75	95	8.22	--
	81118	4,4'-Diamino-2,2'-stilbene-disulfonic acid	7.62/1975/T75	--	--	--
	--	N,N'-Bis(1,4-dimethylpentyl) -p-phenylenediamine	6.06/1974/T74	74 (T74)	4.48	--
B**	91941	3,3'-Dichlorobenzidine base and salts	4.6/1972/T72	125 (T72)	5.77	I, II
M**	1324409	C.I. Pigment Blue 19	4.5/1972/T72	2.39 (T72)	10.72	--
	--	Octyldiphenylamine	2.93/1975/T75 (sales)	82 (T75)	2.39	--

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS (continued)

	CAS No.	Chemical Name	Annual Prod. (Million Pounds)/Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
	--	N,N'-Di-sec-butyl-p-phenylenediamine	2.80/1975/T75	132 (T75)	3.70	--
	90040	o-Anisidine	2.03/1973/T73	148 (delivered)	2.84	--
	--	2-Bromo-4,6-dinitroaniline	2/1974/T74	--	--	--
	4726141	4-(Methylsulfonyl)-2,6-dinitro-N,N-dipropylaniline	2/1972/SRI	--	--	--
M**	101611	4,4'-Methylenebis(N,N-dimethylaniline)	1.86/1974/T74	--	--	I
	4404437	C.I. Fluorescent Brightening Agent 28	1.58/1975/T75	140 (T75)	2.21	--
N**	135886	N-Phenyl-2-naphthylamine	1.56/1975/T75	--	--	I
M	3844459	C.I. Acid Blue 9	1.37/1975/T75	160 (T75)	2.19	--
	91667	N,N-Diethylaniline	1.36/1975/T75	98 (T75)	1.33	--
	12223379	C.I. Disperse Red 60	1.34/1975/T75	381 (T75)	5.09	--
	1861401	N-Butyl-N-ethyl-α,α,α-trifluoro-2,6-dinitro-p-toluidine	1.3/1975/SRI (use)	--	--	--
	74317	N,N'-Diphenyl-p-phenylenediamine	1.07/1975/T75	158 (T75)	1.69	--
	103695	N-Ethylaniline	1.06/1975/T75	84 (tanks)	.89	--

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS (continued)

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[*] Taken from Chemical Marketing Reporter, March 21, 1977, reflecting the list prices prevailing for large lots (f.o.b. New York, unless otherwise indicated). Values designated as coming from Synthetic Organic Chemicals, United States Production and Sales (T74 or T75p, p=preliminary), are unit sales value which is calculated from total quantities sold (the sum of the large quantities sold on a contractual basis and smaller quantities sold intermittently) and total sales value (the sum of the values of sales at contract prices and list prices).

[**] B indicates biphenylamine-related compounds.
M indicates methylenebis (dianiline)-related compounds.
N indicates naphthylamine-related compounds.

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

	CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
	8004873	C.I. Basic Violet 1	996/1975/T75
	--	N,N'-Diisopropyl-p-phenylenediamine	974/1974/T74 (sales)
M**	101779	4,4'-Methylenedianiline	904/1975/T75 (sales)
	81492	1-Amino-2,4-dibromoanthraquinone	857/1974/T74
	--	o-Anisidinomethanesulfonic acid	816/1974/T74
	2475469	C.I. Disperse Blue 3	736/1975/T75
	4208804	C.I. Basic Yellow 11	649/1975/T75
	116814	1-Amino-2-bromo-4-hydroxyanthraquinone	643/1975/T75
	97029	2,4-Dinitroaniline	577/1974/T74
	121471	Metanilic acid	571/1975/T75
	--	C.I. Pigment Red 81 PMA*	505/1975/T75
	--	N^4,N^4-Diethyl-α,α,α-trifluoro-3,5-dinitrotoluene-2,4-diamine	500/1975/SRI (use)
	6408782	C.I. Acid Blue 25	482/1975/T75
	--	1,4-Diamino-2,3-dihydroanthraquinone	470/1975/T75
	6424857	C.I. Acid Blue 40	460/1975/T75
	--	C.I. Pigment Violet 3 PMA*	431/1975/T75
	23422539	m-(((Dimethylamino)methylene)amino)phenyl methyl carbamate, hydrochloride	400/1975/SRI (use)
	5124254	C.I. Disperse Yellow 42	394/1975/T75
	92591	N-Ethyl-N-phenylbenzylamine	383/1975/T75

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

	CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
	1325355	C.I. Direct Orange 15	365/1975/T75
	2787919	C.I. Basic Blue 3	361/1975/T75 (sales)
	2379784	C.I. Vat Orange 15 (10%)	338/1975/T75 (sales)
M**	569642	C.I. Basic Green 4	319/1975/T75
	131920	C.I. Vat Brown 3 (11%)	310/1975/T75
M	--	C.I. Pigment Blue 14 PMA*	284/1974/T74
	3179906	C.I. Disperse Blue 7	271/1975/T75
	1325822	C.I. Pigment Violet 3 (fugitive)	260/1975/T75
	95794	5-Chloro-o-toluidine (NH_2=1)(C.I. Azoic Diazo Component 32)	>251/1972/T72
	4395533	C.I. Vat Black 25 (12.5%)	241/1975/T75
	6359451	C.I. Basic Violet 16	208/1975/T75
	134203	Methyl anthranilate	201/1975/T75
	103060	Anilinomethanesulfonic acid and salt	181/1975/T75
	4403901	C.I. Acid Green 25	171/1975/T75 (sales)
	--	C.I. Vat Blue 6	163.3/1973/T73
	2475458	C.I. Disperse Blue 1	161/1975/T75 (sales)
	82451	1-Aminoanthraquinone and salt	151/1975/T75
	92591	2-(N-Ethylanilino)ethanol	151/1975/T75
	120070	2,2'-((Phenyl)imino)diethanol	128/1975/T75

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

	CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
	--	2,2'-(m-Tolylimino)diethanol	128/1975/T75
M**	2650182	FD & C Blue No. 1	123/1975/T75
M	1694093	C.I. Acid Violet 49	122/1974/T74
	90948	4,4'-Bis(dimethylamino)benzophenone	112/1974/T74
	128869	C.I. Acid Blue 45	112/1975/T75
	--	1((7-Oxo-7H-benz(de)anthracene-3-yl)amino)anthraquinone	103/1975/T75
	--	2,6-Dinitro-N,N-dipropylcumidine	100/1975/SRI (use)
	--	3,5-Dinitro-N^4,N^4-dipropylsulfanilamide	100/1975/SRI (use)
M	2390605	C.I. Basic Blue 7	99/1975/T75
	6408511	C.I. Acid Blue 27	97/1975/T75
	119722	4-Amino-4'-nitro-2,2'-stilbenedisulfonic acid	87/1975/T75
	--	3-(N-Ethyl-m-toluidino)propionitrite	73/1974/T74
	--	C.I. Pigment Violet 1 PTA*	72/1975/T75
M	4680788	C.I. Acid Green 3	71/1975/T75 (sales)
	128950	1,4-Diaminoanthraquinone	70/1974/T74
M	--	C.I. Pigment Blue 1 PMA*	65/1975/T75
	12262509	C.I. Solvent Red 49	64/1975/T75
	--	C.I. Pigment Red 81 PTA*	55/1975/T75
	--	C.I. Pigment Violet 1 PMA*	48/1975/T75
	128950	C.I. Disperse Violet 1	45/1975/T75

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

	CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
	--	2,6-Dibromo-4-nitroaniline	44/1975/T75
	81469	1-Amino-4-benzamidoanthraquinone	43/1974/T74
	116858	C.I. Disperse Red 15	43/1975/T75
	2872482	C.I. Disperse Red 11	42/1974/T74
M**	--	C.I. Acid Green 16	33/1975/T75 (sales)
	--	C.I. Pigment Green 2 PTA*	33/1975/T75
M	3486304	C.I. Acid Blue 7	28/1974/T74 (sales)
	--	C.I. Acid Blue 78	27/1975/T75 (sales)
	--	C.I. Pigment Green 2 PMA*	25/1975/T75 (sales)
	2666173	C.I. Acid Blue 41	20/1975/T75 (sales)
	1220946	C.I. Disperse Violet 4	19/1974/T74 (sales)
	100107	p-(Dimethylamino)benzaldehyde	15/1975/T75
	2379819	C.I. Vat Black 27 (12.5%)	12.5/1975/T75
N**	119777	7-(p-Aminobenzamido)-4-hydroxy-2-naphthalenesulfonic acid	12/1974/T74
	81889	D & C Red No. 19	12/1975/T75
M	4129844	C.I. Acid Violet 17	11/1975/T75 (sales)

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

	CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
M**	--	C.I. Pigment Green 1 PMA*	8/1974/T74
	4368563	C.I. Acid Blue 62	5/1975/T75
M	3943826	C.I. Basic Blue 5	4/1975/T75 (sales)
	87296	Cinnamyl anthranilate	1/1975/T75 (sales)

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[*] PMA = phosphomolybdic acid salt
PTA = phosphotungstic acid salt

[**] M indicates methylenebis (dianiline)-related compounds.
N indicates naphthylamine-related compounds.

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE†

	CAS No.	Chemical Name
	55550	p-Methylaminophenol sulfate
	57670	Sulfaguanidine
	57681	Sulfamethazine
	59405	Sulfaquinoxaline
	61734	Methylene blue
	63741	Sulfanilamide
	65496	Aminosalicylic acid
	68359	Sulfadiazine
	72140	Sulfathiazole
	80080	3,3'-Sulfonyldianiline
	80115	N-Methyl-N-nitroso-p-toluenesulfonamide
	80740	Acetyl sulfisoxazole
N*	81061	1-Amino-2-naphthalenesulfonic acid (o-Naphthionic acid)
N	81163	2-Amino-1-naphthalenesulfonic acid (Tobias acid)
	81425	1,4-Diamino-2,3-dichloroanthraquinone
	81492	1-Amino-2,4-dibromoanthraquinone
	82279	2-Amino-1-chloroanthraquinone
	82382	1-(Methylamino)anthraquinone
	83078 (base)	4-Aminoantipyrene and hydrochloride
N	83238	4-Amino-5-hydroxy-2,7-naphthalenedisulfonic acid, benzenesulfonate
N	83556	5-Amino-1-naphthol
	85916	Methyl-N-methylanthranilate
N	86657	7-Amino-1,3-naphthalenedisulfonic acid (Amino G acid)

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE[†] (continued)

	CAS No.	Chemical Name
	87252	Ethyl anthranilate
	87605	3-Chloro-o-toluidine (NH_2=1)
	88448	6-Amino-m-toluenesulfonic acid (SO_3H=1)
	88517	6-Amino-4-chloro-m-toluenesulfonic acid (SO_3H=1)
	88539	2-Amino-5-chloro-p-toluenesulfonic acid (SO_3H=1)
	88631	2,4-Diaminobenzenesulfonic acid (SO_3H=1)
	88744	o-Nitroaniline
	89269	1-(m-Aminophenyl)-5-oxo-2-pyrazoline-3-carboxylic acid
	89623	2-Nitro-p-toluidine (NH_2=1)
	89634	4-Chloro-2-nitroaniline (p-Chloro-o-nitroaniline)
	90040	o-Anisidine
N*	90302	N-Phenyl-1-naphthylamine
	91236	o-Nitroanisole
	91292	2-(p-Aminoanilino)-5-nitrobenzenesulfonic acid
	91407	N-Phenylanthranilic acid
	91678	N,N-Diethyl-m-toluidine
	91689	m-(Diethylamino)phenol (N,N-Diethvl-3-aminophenol)
	91985	α-(N-Ethyl-m-toluidino)-m-toluenesulfonic acid
	92159	o-Acetoacetanisidide
	92182	N,N-Diethyl-m-anisidine
N	93458	p-(2-Naphthylamino)phenol (N-(p-Hydroxyphenyl)-2-naphthylamine)
N	93469	N,N'-Di-2-naphthyl-p-phenylenediamine

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

CAS No.	Chemical Name
94257	Butyl aminobenzoate
94688	N-Ethyl-o-toluidine
94928	N,N'-Di-o-tolylethylenediamine
95034	5-Chloro-o-anisidine (NH_3=1) (4-Chloro-o-anisidine (OCH_3=1))
95512	o-Chloroaniline
95534	o-Toluidine
95545	o-Phenylenediamine
95556	o-Aminophenol
95681	2,4-Xylidine (m-4-Xylidine)
95692 (base)	4-Chloro-o-toluidine (NH_2=1) and hydrochloride
95749	3-Chloro-p-toluidine (NH_2=1)
95761	3,4-Dichloroaniline
95783	2,6-Xylidine (p-Xylidine)
95729 (base)	2,5-Dichloroaniline and hydrochloride (NH_2=1)
95830	4-Chloro-o-phenylenediamine
95841	2-Amino-p-cresol
96673	2-Hydroxy-5-nitrometanilic acid
96753	2-Amino-5-nitrobenzenesulfonic acid (SO_3H=1)
96968	2-Nitro-p-anisidine (NH_2=1)
97529	4-Nitro-o-anisidine (NH_2=1)
98339	4-Amino-m-toluenesulfonic acid (SO_3H=1)
98362	4-Chlorometanilic acid

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

	CAS No.	Chemical Name
	98373	4-Hydroxymetanilic acid
	98431	4-Sulfoanthranilic acid
	98442	2-Amino-p-benzenedisulfonic acid
	99036	3'-Aminoacetophenone
	99070	m-(Dimethylamino)phenol
	99309	2,6-Dichloro-4-nitroaniline
	99558	5-Nitro-o-toluidine (NH_2=1)
	99569	4-Nitro-o-phenylenediamine
	99989	N,N-Dimethyl-p-phenylenediamine
	100174	p-Nitroanisole
	101111	α-(N-Ethylanilino)-m-toluenesulfonic acid
M*	101144	4,4-Methylenebis(2-chloroaniline)
	101188	m-Anilinophenol
	101542	N-Phenyl-p-phenylenediamine
	101702	4,4'-Dimethoxydiphenylamine
	101724	N-Isopropyl-N'-phenyl-p-phenylenediamine
	101735	4-Isopropoxydiphenylamine
	102012	Acetoacetanilide
	102567	2,5-Dimethoxyaniline
	103968	N,N'-Bis(1-methylheptyl)-p-phenylenediamine
	104949	p-Anisidine
	106401	p-Bromoaniline
	106478	p-Chloroaniline

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

	CAS No.	Chemical Name
	106490	p-Toluidine
	106503	p-Phenylenediamine
	108429	m-Chloroaniline
	108441	m-Toluidine
	108452	m-Phenylenediamine
N*	116632	4-Amino-3-hydroxy-1-naphthalenesulfonic acid (1,2,4-acid)
B*	117613	4,4'-Diamino-2,2'-biphenyldisulfonic acid
N	118332	6-Amino-1,3-naphthalenedisulfonic acid (Amino I acid)
N	118445	N-Ethyl-1-naphthylamine
	118923	Anthranilic acid
	119153	p-(2,4-Dinitroanilino)phenol
N	119404	7-Anilino-4-hydroxy-2-naphthalenesulfonic acid (Phenyl J acid)
	119700	5'-Amino-2-(p-aminoaniline)benzenesulfonic acid
	119755	Nitrodiphenylamine
B	119904	3,3'-Dimethoxybenzidine (o-Dianisidine)
B	119937	3,3'-Dimethylbenzidine (o-Tolidine)
	120218	p-(Diethylamino)benzaldehyde
	120354	3-Amino-p-anisanilide
	120376	3-(Ethylamino)-p-cresol
	120718	5-Methyl-o-anisidine (NH_2=1)
	121302	4-Amino-6-chloro-m-benzenedisulfonamide
	121573	Sulfanilic acid (p-aminobenzenesulfonic acid)
	121879	2-Chloro-4-nitroaniline (o-Chloro-p-nitroaniline)

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

	CAS No.	Chemical Name
	122112	Sulfadimethoxine
	122805	4'-Aminoacetanilide
	122985	2-Anilinoethanol
	123308	p-Aminophenol
	127560	Sulfacetamide, sodium
	127582	Sulfamerazine, sodium
	127695	Sulfisoxazole
	127719	Sulfabenzamide
	127797	Sulfamerazine
	128836	1-Amino-2-bromo-4-p-toluidinoanthraquinone
	128869	4,8-Diamino-9,10-dihydro-1,5-dihydroxy-9,10-dioxo-2,6-anthracenedisulfonic acid
	128870	1,1'-Iminobis(4-aminoanthraquinone)
	129442 (1,5)	1,5(and 1,8)-Diaminoanthraquinone
	129420 (1,8)	
N*	130132	4-Amino-1-naphthalenesulfonic acid, sodium salt
	130176 (base)	2-(p-Aminophenyl)-6-methyl-7-benzothiazolesulfonic acid and salt
	131146	2,6-Diaminoanthraquinone
N	131271	3-Amino-1,5-naphthalenedisulfonic acid (C acid)
	132321	3-Amino-9-ethylcarbazole
	133108	Sodium aminosalicylate
	134098	Menthyl anthranilate
	134203	Anthranilic acid, methyl ester
N	134327	1-Naphthylamine (α-Naphthylamine)

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

	CAS No.	Chemical Name
M*	135911	4,4'-Methylenebis(N,N-diethylaniline)
	136801	2-o-Toluidinoethanol
	137075	o-Aminobenzenethiol
	138396	α-Amino-p-toluenesulfonamide
	139606	N,N'-Bis(1-ethyl-3-methylpentyl)-p-phenylenediamine
	140283	N,N'-Dibenzylethylenediamine
	144741	Sulfathiazole, sodium
	144809	Sulfacetamide
	144821	Sulfamethizole
	144832	Sulfapyridine
	145493	1,5-Diamino-4,8-dihydroxyanthraquinone
	150130	p-Aminobenzoic acid
	150618	N,N'-Diphenylethylenediamine
	156105	4-Nitrosodiphenylamine
	156434	p-Phenetidine
	535875	3,5-Diaminobenzoic acid
	536470	N,N-Dimethyl-p-phenylenediamine sulfate
	540238	p-Toluidine hydrochloride
	540249	p-Phenylenediamine hydrochloride
M**	548629	Gentian Violet
	577480	Butamben picrate
	723466	Sulfamethoxazole
	967806	Sulfaquinoxaline, sodium

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

	CAS No.	Chemical Name
	1323064	N-Cyclohexyl-N'-phenyl-p-phenylenediamine
	1752245	p-Hydroxydiphenylamine
	1861401	N-Butyl-N-ethyl-α,α,α-trifluoro-2,6-dinitro-p-toluidine (Benefin)
	1981584	Sulfamethazine, sodium
	2052462	N,N-Dimethyl-p-phenylenediamine monohydrochloride
	2465272	Auramine o
	4726141	4-(Methylsulfonyl)-2,6-dinitro-N,N-dipropylaniline (Nitralin)
N*	5959524	3-Amino-2-naphthoic acid
	6358641	4-Chloro-2,5-dimethoxyaniline
	7149260	3,7-Dimethyl-1,6-octadien-3-yl,anthranilate
	7257445	Sulfabenzamide, sodium
	12041677	Ethyl aminobenzoate (Benzocaine)
	--	Acetaldehyde-aniline condensate
	--	2,2'((3-Acetamido-6-ethoxyphenyl)imino)diethanol
	--	2,2'((5-Acetamido-2-ethoxyphenyl)imino)diethanol
	--	α-Acetylamino-p-toluenesulfonamine
	--	N-Acetylanthranilic acid
	--	3'-Aminoacetanilide
	--	3'-Amino-p-acetphenetidine
	--	3'-Amino-p-acetanisidide
	--	1-Amino-4-(3-amino-4-sulfoanilino)-9,10-dihydro-9,10-dioxo-2-anthracenesulfonic acid
	--	5(and 8)-Amino-8(and 5)-bromo-9,10-dihydro-9,10-dioxo-1,6(and 1,7)-anthracenedisulfonic acid
	--	1-Amino-4-bromo-9,10-dihydro-9,10-dioxo-2-anthracenesulfonic acid and sodium salt
	--	2-Aminoanthraquinone and salt

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

	CAS No.	Chemical Name
	--	o-Aminobenzamide
	--	p-Aminobenzamide
	--	3'-Aminobenzanilide
	--	1-Amino-5-chloroanthraquinone
	--	4-Amino-6-chloro-m-benzenedisulfonamide hydrochloride
	--	2-Amino-5-chloro-4-ethylbenzenesulfonic acid
	--	1-Amino-2-chloro-4-hydroxyanthraquinone
	--	1-(2-Amino-5-chlorophenyl)-1-phenyl methylenimine
	--	1-Amino-2,4-dichloroanthraquinone
	--	3-Amino-2,5-dichlorobenzoic acid, ammonium salt
	--	3-Amino-2,5-dichlorobenzoic acid, methyl ester
	--	2-Amino-4,6-dichloro-5-cresol
	--	1-Amino-9,10-dihydro-9,10-dioxo-4-p-toluenesulfonamido-2-anthracenesulfonic acid, sodium salt
	--	4-Amino-N,N-dihydroxyanisole
	--	3-Amino-α-ethylhydrocinnamic acid
	--	4-Amino-N-ethyl-N-(β-methylsulfonamidoethyl)-m-toluidine phosphate
	--	N-(2-(4-Amino-N-ethyl-m-toluidino)ethyl)methanesulfonamide
	--	2-(4-Amino-N-ethyl-m-toluidino)ethyl sulfate
N*	--	4-Amino-5-hydroxy-2,7-naphthalenedisulfonic acid (H acid), monosodium salt
N	--	6-Amino-4-hydroxy-2-naphthalenesulfonic acid (Gamma acid), sodium salt
N	--	7-Amino-4-hydroxy-2-naphthalenesulfonic acid (J acid), sodium salt
	--	3-Amino-2-hydroxy-5-nitroacetanilide
	--	3-Amino-2-mercaptobenzoic acid

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

	CAS No.	Chemical Name
	--	4-Amino-3-(β-methanesulfonamidoethyl)-N,N-diethylaniline hydrochloride
	--	3-Amino-4-methoxybenzenesulfonic acid
N*	--	5-Amino-6-methoxy-2-naphthalenesulfonic acid
	--	2-Amino-4-methoxytoluene
	--	2-Amino-4'-methyldiphenylsulfone-4-sulfonic acid
	--	2-Amino-4-(methylsulfonyl)phenol
N	--	2-Amino-1,5-naphthalenedisulfonic acid
N	--	7-Amino-1,3,5-naphthalenetrisulfonic acid
N	--	7-Amino-1,3,6-naphthalenetrisulfonic acid
N	--	8-Amino-1,3,6-naphthalenetrisulfonic acid (Koch's acid)
N	--	8-Amino-2-naphthol
N	--	5-Amino-2-naphthol
	--	2-Amino-4-nitroacetanilide
	--	3-Amino-5-(m-nitrobenzamide)-p-toluenesulfonic acid
	--	2-Amino-4-(1,1,3,3-tetramethylbutyl)phenol, crude
	--	2-Amino-4-(1,1,3,3-tetramethylbutyl)phenolhydrochloride
	--	3-Amino-p-toluamide
	--	Amyl-p-dimethylaminobenzoate
	--	2'-Anilino-6-diethylamino-3-methylfluoran
	--	1-Anilino-9,10-dihydro-9,10-dioxo-2-anthroic acid
	--	p-Anilinophenol
	--	Antidegradant 64
	--	Antidegradant 66

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

	CAS No.	Chemical Name
	--	Antidegradant 67
	--	Benzoic acid, 3-(N-(2-hydroxyethyl)anilino)propionitrile ester
B*	--	Benzidine base
B	--	4,4'-Benzylidenedi-o-toluidine
B	--	(1,1-Biphenyl)-4,4'-diamine dihydrochloride
	--	3'-(Bis(2-acetoxyethyl)amino)-p-acetoanisidide
	--	1,4-Bis(1-anthraquinonylamino)anthraquinone
	--	1,4-Bis(1-anthraquinonylamino)anthraquinone and 1,4-Bis-(5-chloro-1-anthraquinonylamino)anthraquinone (mixed)
	--	N,N-Bis(cyanoethyl)aniline
	--	N,N-Bis(1,4-dimethylpentyl)-p-phenylenediamine
	--	3'-(Bis(2-hydroxyethyl)amino)acetanilide
	--	2,4-Bis(n-octylthio)-6-(4'-hydroxy-3',5'-di-tert-butylanilino)-1,3,5-triazine
	--	2-Bromo-6-chloro-4-nitroaniline
	--	n-Butraldehyde-aniline condensate
	--	p-Butylaminobenzoic acid, ethyl ester
	--	3-(N-Butylanilino)propionitrile
	--	N-sec-Butyl-N'-phenyl-p-phenylenediamine
	--	2-(o-chloroanilino)ethanol
	--	3-(o-Chloroanilino)propionitrile
	--	2-Chloro-N,N-diethyl-4-nitroaniline
	--	3-Chlorodiphenylamine

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

CAS No.	Chemical Name
--	N-(2-Chloroethyl)-N-ethylaniline
--	2-Chloro-4-ethylmetanilic acid
--	1-(p-Chlorophenyl)-3-methyl-n-ethylaniline
--	2-(N-Cyclopropylmethyl-N-phthalimidoacetyl) amino-5-chlorobenzophenone
--	3-(Di-(2-acetoxyethyl)amine)-p-acetophenetidide
--	2,5-Diaminobenzenesulfonic acid ($SO_3H=1$)
--	4'4'-Diamino-1,1'-bianthraquinene-3,3'-disulfonic acid, disodium salt
--	1,4-Diamino-9,10-dihydro-9,10-dioxo-2,3-anthracenedicarboximide
--	3,5-Diamino-2,4,6-triiodobenzoic acid
--	Dianisidine diisocyanate (DADI)
--	Diaryl-p-phenylenediamine
--	N,N'-Dibenzylethylenediamine diacetate
--	2,6-Dibromo-4-nitroaniline
--	2,6-Di-tert-butyl-α-dimethylamino-p-cresol
--	N,N'-Di-sec-butyl-o-phenylenediamine
--	3-(2,4-Dichloroanilino)-1-(2,4,6-trichlorophenyl)-2-pyrazolin-5-one
--	N,N'-Dicyclohexyl-p-phenylendiamine
--	3'-(2-(Diethylamino)ethyl)-4'-hydroxyacetanilide
--	7'-Diethylamino-4-methylcoumarin
--	4-(Diethylamino)-o-tolualdehyde
--	2,6-Diethylaniline
--	N,N-Diethyl-4-nitroso-m-anisidine hydrochloride

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

	CAS No.	Chemical Name
	--	N,N-Diethyl-4-nitroso-m-phenetidine
	--	N,N-Diethyl-m-phenetidine
	--	N,N-Diethyl-p-phenylenediamine hydrochloride
	--	N,N-Diethyltoluene-2,5-diamine, monohydrochloride
	--	N^4,N^4-Diethyl-α,α,α-trifluoro-3,5-dinitro-toluene-2,4-diamine (Dinitroamine)
B*	--	3,3'-Dimethoxybenzidine hydrochloride
	--	p-Dimethylaminobenzenediazonium chloride
	--	m-(Dimethylamino)benzoic acid
	--	6-Dimethylamino-2-(2,5-dimethyl-1-phenyl-3-pyrryl)-vinyl)-1-methyl-1-quinolinium methyl sulfate
	--	6-Dimethylamino-1-methylquinaldinium methyl sulfate
	--	6-Dimethylaminoquinaldine
B	--	3,3'-Dimethylbenzidine hydrochloride
	--	N,N-Dimethyl-p-toluidine
	--	N,N-Dimethyl-o-toluidine
	--	Diphenylamine-acetone condensate
	--	p-Diphenylaminodiazonium sulfate
	--	Diphenylamine, styrenated
	--	N,N'-Diphenyl-1,3-propanediamine
	--	1,5-Di-p-toluidinoanthraquinone
	--	N-(p-Ethoxybenzylidene)-p-butylaniline
	--	N-Ethyl-N-(β-aminoethyl)-m-toluidine
	--	3-(Ethylamino)-p-toluenesulfonic acid (SO_3H=1)

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

CAS No.	Chemical Name
--	(2-(N-Ethylanilino)ethyl)trimethylammonium chloride
--	1-(2-(Ethylanilino)ethylene)pyridinium chloride
--	3-(N-Ethylanilino)propionitrile
--	α-(N-Ethylanilino)-p-toluenesulfonic acid
--	N-Ethyl-N-(2-chloroethyl)aniline
--	2-(N-Ethyl-N-β-cyanoethyl)-4-acetaminoanisole
--	N-Ethyl-N-glycerol-m-toluidine
--	2-Ethylhexyl-p-dimethylaminobenzoate
--	N-Ethyl-N-hydroxyethyl-p-phenylenediamine sulfate
--	N-Ethyl-N-(β-methylsulfonamidoethyl)-m-toluidine
--	N-Ethyl-m-toluidine
--	2-(N-Ethyl-m-toluidino)ethanol
--	Heptaldehyde-aniline condensate
--	Hydroxycitronellalmethyl anthranilate
--	3-(N-(2-Hydroxyethyl)anilino)propionitrile
--	3-(N-(2-Hydroxyethyl)anilino)propionitrile, acetate
--	3-(N-(2-Hydroxyethyl)anilino)propionitrile, benzoate
--	P(2-hydroxyethyl)methylamino)benzenediazonium chloride
--	Isobutyl aminobenzoate
--	2-Methoxy-5-acetamino-N,N-bis(acetoxyethyl)aniline
--	N-(p-Methoxybenzylidene)-p-butylaniline
--	3-(N-Methylanilino)propionitrile

Class: Aromatic Amines

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

	CAS No.	Chemical Name
	--	5-Methyl-o-anisidinesulfonic acid
	--	m-Methylanisole
	--	N-Methylanthranilic acid
	--	N-Methyleneaniline
M*	--	4,4'-Methylenediamine salt complex
	--	α-Methyl-p-isopropyl hydrocinnamaldehyde methyl anthranilate (Orangeol N)
	--	4-Methyl-2-nitroanisole
	--	N-(1-Methylpentyl)-N'-phenyl-p-phenylenediamine
	--	5-Nitroanthranilic acid
	--	p-Nitrodimethylaminoethylbenzoate
	--	4-Nitroso-N-ethyl-N(β-methylsulfonamidoethyl)-m-toluidine
	--	Nonyldiphenylamine mixture (mono-, di-, and tri-)
	--	Octyldiphenylamine, alkylated
	--	Octyldiphenylamine mixture (mono-, di-, and nonyl-)
	--	N-Phenyl-N-sec-butyl-o-phenylenediamine
N*	--	Phenyl-2-naphthylamineacetone condensate
	--	N-Phenyl-N'-2-octyl-p-phenylenediamine
	--	Sulfabromomethazine, sodium
	--	Sulfachloropyrazine, sodium
	--	Sulfachloropyridazine, sodium
	--	3,3',4,4'-Tetraaminobenzophenone

AROMATIC AMINES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE[†] (continued)

CAS No.	Chemical Name
--	4,4',4",4"'-Tetraaminophthalocyaninato(2-))copper
--	N,N,N',N'-Tetramethyl-p-phenylenediamine dihydrochloride
--	p-(p-Toluenesulfonamido)diphenylamine
--	o-Toluidine hydrochloride
--	o-Toluidinomethanesulfonic acid
--	N,N,N-Tribenzylamine

[†] Compiled from Synthetic Organic Chemicals, United States Production and Sales, 1975, excluding the Dyes and Pigments sections. Because of the large number of chemicals listed in these sections on dyes and pigments for which exact structures would have to be determined, these have not been included in this table. Chemicals from the section on medicinals were included only if an initial examination of the names listed indicated that they fit the category. CAS Numbers were included only if found in one search of readily available sources.

** B indicates biphenylamine-related compounds.
M indicates methylenebis (dianiline)-related compounds.
N indicates naphthylamine-related compounds.

8. Class VIII: Azo Compounds

The chemicals in this class are those with a known or estimated annual production level of one million pounds or more. These chemicals can be divided into two major use categories: dyes and pigments. Dyes are coloring materials in solution. Pigments are coloring materials in suspension.

Dyes

There are six chemicals in this use category: (1) C.I. Disperse Yellow 3; (2) C.I. Disperse Blue 79; (3) C.I. Direct Black 38; (4) C.I. Acid Yellow 151; (5) FD & C Yellow No. 5; and (6) C.I. Direct Blue 218.

Production, use, and growth trends are discussed separately for each dye. Possible chemical substitutes for these dyes can only be discussed in general terms. Besides economic considerations, choosing a specific substitute for a particular dye depends on many physical and technical properties of the dye that affect its usage in specific products, e.g., hue, dyeing properties, application methods, substrates, fastness properties, etc. Although many possible substitute dyes exist, the choice of these substitutes would rest with a technical dye expert.

C.I. Disperse Yellow 3

In 1975, U.S. production of C.I. Disperse Yellow 3 amounted to 3.125 million pounds, an increase of 8.8% over the 1974 production level of 2.87 million pounds. However, in 1974, production had declined 23.5% over the 1973 production high of 3.748 million pounds. During the period 1970-1973, C.I. Disperse Yellow 3 production had grown at an average annual rate of 26%. Imports of C.I. Disperse Yellow 3 through principal U.S.

customs districts amounted to only 1,517 pounds in 1975. U.S. exports data for this chemical are not published separately.

C.I. Disperse Yellow is used to dye acetate, nylon, triacetate, polyester, acrylic, and polyvinyl chloride fibers. It is an important component for hosiery shades, and is also used to dye wool sheepskins and furs, and in the surface dyeing of cellulose acetate, polymethyl methacrylate, and other plastics. Future growth of disperse dyes, including C.I. Disperse Yellow 3, is tied to growth in the polyester fiber market, and is expected to bounce back from the recent recession and continue to grow beyond 1985.

C.I. Disperse Blue 79

Production of C.I. Disperse Blue 79 was reported as 3.023 million pounds in 1975, a decrease of 38.5% from a production high of 4.91 million pounds in 1974. C.I. Disperse Blue 79 production had grown at an average annual rate of 36% during the period 1970-1974. U.S. imports of C.I. Disperse Blue 79 through principal U.S. customs districts amounted to 45,591 lbs. in 1975. U.S. exports data for this chemical are not available.

C.I. Disperse Blue 79 is used to dye triacetate and polyester fibers. Future growth of disperse dyes, including C.I. Disperse Blue 79, is tied to growth in the polyester fiber market, which is expected to bounce back from the recent recession and continue to grow beyond 1985.

C.I. Direct Black 38

In 1975, U.S. production of C.I. Direct Black 38 amounted to 2.168 million pounds, a decrease of more than 200% from the 1973 production level of 6.743 million pounds. U.S. imports and exports data are not published separately for this chemical.

C.I. Direct Black 38 is used to dye cellulose, wool, silk, bast fibers, hog's hair, and leather. It is used for printing on cellulose, wool, and silk. It is also used as a colorant in aqueous inks, plastics, wood stains, vegetable-ivory buttons, as a biological stain, and to color wood-flour used as a resin filler. In general, cellulosic dyestuff consumption is expected to decline after 1977.

C.I. Acid Yellow 151

Production of C.I. Acid Yellow 151 amounted to 1.738 million pounds in 1975, down from a production high of 1.799 million pounds in 1973. U.S. imports and exports data are not available for this chemical.

C.I. Acid Yellow 151 is used to dye wool and silk and for printing on wool, silk, and nylon. Growth of acid dyes, including C.I. Acid Yellow 151, is expected to increase as demand for nylon carpet increases with new housing starts.

FD & C Yellow No. 5

Production of FD & C Yellow No. 5 amounted to 1.070 million pounds in 1975, down from a production high of 1.525 million pounds in 1974. C.I. Acid Yellow 23 is chemically identical with FD & C Yellow No. 5 and differs only in purity specifications or product form. Production of C.I. Acid Yellow 23 amounted to 271 thousand pounds in 1975, down from 336 thousand pounds in 1974, and a production high of 631 thousand pounds in 1973. U.S. imports of FD & C Yellow No. 5 and C.I. Acid Yellow 23 through principal U.S. customs districts amounted to 281,358 lbs. and 6,240 lbs., respectively, in 1975. U.S. exports data are not available for these chemicals.

Certified FD & C Yellow No. 5 is approved for use as a color additive in food, drugs, and cosmetics by the U.S. Food and Drug Administration. Based on U.S. sales data for the first nine months of 1967, FD & C Yellow No. 5 was used to color food (96%), pharmaceuticals (3%) and cosmetics (1%). Based on these data, a breakdown for the consumption of FD & C Yellow No. 5 in food during this period was: pet food (18.8%); beverages (14.6%); bakery goods (14.4%); dessert powders (11.1%); candy and confections (11.1%); cereals (9.7%); miscellaneous foods (8.2%); ice cream, sherbet, and dairy products (6.5%); snack foods (3.4%); sausage (1.2%); and maraschino cherries (1.0%).

As a drug color additive, FD & C Yellow No. 5 has been used in aqueous drug solutions, tablets, and capsules. As a cosmetics color additive, FD & C Yellow No. 5 has been used in toothpaste, hair waving fluids, and bath salts, and its aluminum lake has been used in lipsticks, rouges, face and talcum powders, and nail lacquers.

The U.S. Food and Drug Administration is currently proposing that FD & C Yellow No. 5 be prohibited from use in the following drugs: pain relievers, antihistamines, cough-cold medications, anti-asthmatics, orally administered decongestants, and prescription anti-inflammatory drugs. It is also proposing that labels of any food products containing FD & C Yellow No. 5 should specifically list it as an ingredient. These restrictions and requirements result from the probability that as many as 100,000 Americans have allergic reactions to FD & C Yellow No. 5.

Possible substitutes for FD & C Yellow No. 5 include the only other synthetic yellow food color approved by the FDA, FD & C Yellow No. 6, various natural derivatives, and a new polymeric food dye (which is not absorbed by the bloodstream) which may be introduced to the marketplace by 1980.

C.I. Acid Yellow 23 is used to dye wool, silk, nylon, and leather; for printing on wool and silk; as a stain and surface color for crepe tissues; to color soap, casein plastics, anodized aluminum, writing inks, and woodstains. Growth of acid dyes, including C.I. Acid Yellow 23, is expected to increase as demand for nylon carpet increases with new housing starts.

C.I. Direct Blue 218

U.S. production of C.I. Direct Blue 218 amounted to 1.045 million pounds (with sales of 1.309 million pounds) in 1975. Production of this dyestuff peaked in 1973, when it reached 1.472 million pounds. U.S. imports and exports data for this chemical are not published separately.

C.I. Direct Blue 218 is used to dye cellulose, stain silk and wool, and is suitable for use on goods to be given a urea-formaldehyde finish. In general, cellulosic dyestuff consumption is expected to decline after 1977.

Pigments

There are nine chemicals in this use category: (1) C.I. Pigment Yellow 12; (2) C.I. Pigment Red 49, barium toner; (3) C.I. Pigment Red 49, calcium toner; (4) C.I. Pigment Red 53, barium toner; (5) C.I. Pigment Red 48; (6) C.I. Pigment Red 52; (7) C.I. Pigment Yellow 14; (8) C.I. Pigment Red 3; and (9) C.I. Pigment Red 57, calcium toner.

Production and use descriptions are presented separately for each pigment. Possible chemical substitutes for these pigments can only be discussed in general terms. Besides economic considerations, choosing a specific substitute for a particular pigment depends on many physical and technical properties of the pigment that affect its usage in specific products, e.g., hue, tinctorial strength, ease of incorporation into the medium, transparency or opacity, fastness, solubility in various solvents, etc. Although many possible substitute pigments exist, the choice of these substitutes would rest with a technical pigments expert.

Pigment sales in 1976 are believed to have reached 1973 levels, recovering from the 1974-1975 slump. The general outlook for the organic pigment industry is good. Pressures on lead pigment users stemming from possible government regulations may result in increased organic pigment sales. Estimated annual growth rates are not available.

C.I. Pigment Yellow 12

In 1975, C.I. Pigment Yellow 12 production amounted to 6.028 million pounds, a decrease of 25% over the 1974 production level of 8.019 million pounds. A production high for C.I. Pigment Yellow 12 of 8.398 million pounds was reported in 1973. Imports of C.I. Pigment Yellow 12 through principal U.S. customs districts amounted to 62 thousand pounds in 1975. U.S. exports data for this chemical are not available.

C.I. Pigment Yellow 12 is used in: printing inks and lacquers; rubber; polyvinyl chloride, urea/formaldehyde, and phenol/formaldehyde resins; paper; textile printing; and linoleum.

C.I. Pigment Red 49, barium toner, and C.I. Pigment Red 49, calcium toner

Production of C.I. Pigment Red 49, barium toner, dropped 16% in 1975 to 4.015 million pounds from a 1974 level of 4.787 million pounds. During the 1970-1975 period, annual production of C.I. Pigment Red 49, barium toner, remained in the range of 4.0-4.8 million pounds per year. Imports of

C.I. Pigment Red 49, barium toner, through principal U.S. customs districts amounted to 17 thousand pounds in 1975.

C.I. Pigment Red 49, barium toner, is chemically identical to D & C Red No. 12. In 1975, U.S. production of D & C Red No. 12 amounted to only 5,000 pounds.

In 1975, production of C.I. Pigment Red 49, calcium toner, amounted to 1.297 million pounds. During the period 1970-1975, annual production of C.I. Pigment Red 49, calcium toner, has remained within a range of 1.25-1.431 million pounds per year (the peak, 1.431 million pounds, was reported in 1970). U.S. imports data for this chemical are not available.

D & C Red No. 11 is chemically identical to C.I. Pigment Red 49, calcium toner. At least 1,000 pounds of D & C Red No. 11 were produced in the U.S. in 1975 but separate data are not published.

U.S. exports data for these chemicals are not available.

C.I. Pigment Red 49, barium toner and calcium toner, have identical uses. They are primarily used because they are inexpensive; however, they cannot be used where the pigmented product is subjected to severe conditions. They are used in printing inks and paints having high tinctorial strength; in alkyd resin enamels and lacquers when the solvent fastness is sufficient; in rubber (although migration may occur); in linoleum, paper coating, and student-grade artists' coloring materials; and in polyvinyl chloride, urea/formaldehyde, phenol/formaldehyde, polystyrene, and amino resin and plastics.

D & C Red No. 12 and D & C Red No. 11 are used in powders, rouges, lipsticks, creams, nail lacquers, and soap.

C.I. Pigment Red 53, barium toner

Production of C.I. Pigment Red 53, barium toner, dropped 25% in 1975 to 2.736 million pounds from a production high of 3.656 million pounds in 1974. Annual production of C.I. Pigment Red 53, barium toner, increased at an average rate of 13.9% during the period 1970-1974. Imports of C.I. Pigment Red 53, barium toner, through principal U.S. customs districts amounted to 13 thousand pounds in 1975. U.S. exports data for this chemical are not available.

C.I. Pigment Red 53, barium toner, is chemically identical to D & C Red No. 9. In 1975, production of D & C Red No. 9 amounted to 62 thousand pounds.

C.I. Pigment Red 53, barium toner, is used in printing inks (sheet-fed and webb offset heat-set and flexographic), in coated paper, crayons, rubber, polystyrene, polyvinyl chloride, urea/formaldehyde and phenol/formaldehyde resins and plastics, and baking enamels.

D & C Red No. 9 is used in powders, rouges, lipsticks, creams, nail lacquers, and soap.

C.I. Pigment Red 48

Annual production of C.I. Pigment Red 48 has declined from a production high of 3.48 million pounds in 1972 to a 1975 production level of 2.167 million pounds. The largest decline occurred in 1974, when annual production dropped 23%. Imports of C.I. Pigment Red 48 through principal U.S. customs districts amounted to 171 thousand pounds in 1975. U.S. exports data for this chemical are not available.

C.I. Pigment Red 48 as the barium or calcium salt is used primarily in printing inks and plastics. It is used in printing inks of high tinctorial strength, wrapper and tinplate printing inks, and in textile printing. It finds use in the following plastics: polyvinyl chloride, urea/formaldehyde, and phenol/formaldehyde. Other applications for C.I. Pigment Red 48, barium and calcium salts, are in paints, alkyd resin enamels and lacquers, rubber, paper, linoleum, book cloth, leather cloth, and cosmetics.

C.I. Pigment Red 48, manganese salt, is used primarily in paints, alkyd resin enamels, lacquers, plastics, and vinyl products. It is also used occasionally in emulsion paints, printing inks, paper, and textile printing, and only occasionally in rubber.

C.I. Pigment Red 52

In 1975, production of C.I. Pigment Red 52 amounted to 1.93 million pounds. During the period 1970-1975, annual C.I. Pigment Red 52 production remained in the range of 1.55-1.93 million pounds per year. Imports of C.I. Pigment Red 52 through principal U.S. customs districts amounted to only 1,764 pounds in 1975. U.S. exports data for this chemical are not available.

C.I. Pigment Red 52, calcium salt, is used in printing inks, plastics, rubber, enamels, lacquers, floor coverings, and sometimes in emulsion paints.

C.I. Pigment Red 52, manganese salt, is primarily used in paints, with additional applications as described for the calcium salt.

C.I. Pigment Yellow 14

Production of C.I. Pigment Yellow 14 decreased 49% in 1975, to 1.84 million pounds, from a production high of 3.60 million pounds in 1974. Annual production of C.I. Pigment Yellow 14 remained in the range of 1.84-3.60 million pounds per year, during the period 1970-1975. Imports of

C.I. Pigment Yellow 14 through principal U.S. customs districts amounted to 11 thousand pounds in 1975. U.S. exports data for this chemical are not available.

C.I. Pigment Yellow 14 is used in: rubber; urea/formaldehyde, phenol/formaldehyde, polyvinyl chloride, polystyrene, and vinyl plastics; printing inks; and for textiles. It is occasionally used in paints and paper.

C.I. Pigment Red 3

Production of C.I. Pigment Red 3 dropped 26% from a production high in 1974 of 2.24 million pounds to 1.66 million pounds in 1975. Annual C.I. Pigment Red 3 production stayed in the range of 1.626-2.24 million pounds per year during the period 1970-1975. Imports of C.I. Pigment Red 3 through principal U.S. customs districts amounted to 105 thousand pounds in 1975. U.S. exports data for this chemical are not available.

C.I. Pigment Red 3 is one of the most widely used red pigments due to its coloring properties and economic considerations. It is primarily used in paints (trim paints, bulletin paints, farm machinery finishes, emulsion paints). Small amounts are used in printing inks (mainly poster inks). Other applications include: distempers, synthetic resin lacquers and leather finishes, paper coating and dyeing, wallpaper, linoleum, carbon paper, typewriter ribbon, student-grade art materials, cement, and textile printing. C.I. Pigment Red 3 can also be used in rubber, celluloid, cellulose acetate, phenol/formaldehyde, urea/formaldehyde, styrene, and protein plastics; however, migration may occur or other physical conditions may make this usage impractical.

C.I. Pigment Red 57, calcium toner

Production of C.I. Pigment Red 57, calcium toner, has declined slightly from a 1973 high of 1.578 million pounds (with a 1.6% decline in 1974 and a further 3.7% decline in 1975) to a 1975 production level of 1.496 million pounds. Annual production of C.I. Pigment Red 57, calcium toner, has stayed in the range of 1.023-1.578 million pounds per year during 1970-1975. Imports of C.I. Pigment Red 57, calcium toner, through principal U.S. customs districts amounted to 330 thousand pounds in 1975. U.S. exports data for this chemical are not available.

C.I. Pigment Red 57, calcium toner, is chemically identical to D & C Red No. 7. In 1975, U.S. production of D & C Red No. 7 amounted to 20 thousand pounds.

C.I. Pigment Red 57, calcium toner, is used primarily in printing inks. It also has important usage in paints, alkyd resin enamels, lacquers, rubber, and vinyl products. Other uses include: paper coatings, wallpaper, linoleum, most types of plastics, leather finishes, and textile printing.

D & C Red No. 7 is used in powders, rouges, lipsticks, creams, nail lacquers, and soap.

Class: Azo Compounds

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE MILLION POUNDS

CAS No.	Chemical Name	Annual Prod. (Million Pounds)/Year/Source	Price*, ¢/lb.	Market Value, Million $	Dossiers
6358856	C.I. Pigment Yellow 12	6.03/1975/T75	335 (T75)	20.19	--
1103384	C.I. Pigment Red 49, barium toner	4.02/1975/T75	212 (T75)	8.51	--
2832408	C.I. Disperse Yellow 3	3.13/1975/T75	198 (T75)	6.19	I, II
12239348	C.I. Disperse Blue 79	3.02/1975/T75	266 (T75)	8.04	--
5160021	C.I. Pigment Red 53, barium toner	2.74/1975/T75	270 (T75)	7.39	I, II
1937377	C.I. Direct Black 38	2.17/1975/T75	--	--	--
3564214	C.I. Pigment Red 48	2.17/1975/T75	394 (T75)	8.54	--
5858822	C.I. Pigment Red 52	1.93/1975/T75	366 (T75)	7.06	--
5468757	C.I. Pigment Yellow 14	1.84/1975/T75	349 (T75)	6.42	--
--	C.I. Acid Yellow 151	1.74/1975/T75	233 (T75)	4.05	--
2425856	C.I. Pigment Red 3	1.66/1975/T75	331 (T75)	5.49	--
5281049	C.I. Pigment Red 57, calcium toner	1.5/1975/T75	405 (T75)	6.06	--
1103395	C.I. Pigment Red 49, calcium toner	1.3/1975/T75	243 (T75)	3.15	--
1934210	FD & C Yellow No. 5	1.07/1975/T75	498 (T75)	5.33	I
10401500	C.I. Direct Blue 218	1.05/1975/T75	230 (T75)	2.40	--

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*Values designated as coming from Synthetic Organic Chemicals, United States Production and Sales (T74 or T75p, p=preliminary), are unit sales value which is calculated from total quantities sold (the sum of the large quantities sold on a contractual basis and smaller quantities sold intermittently) and total sales value (the sum of the values of sales at contract prices and list prices).

Class: Azo Compounds

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
6358312	C.I. Pigment Yellow 74	947/1975/T75
--	C.I. Direct Yellow 50[1]	942/1975/Tp75
2783940	FD & C Yellow No. 6	804/1975/T75
3734676	C.I. Acid Red 1	798/1975/T75
842079	C.I. Solvent Yellow 14	783/1975/T75
915673	FD & C Red No. 2	680/1975/T75
6371842	C.I. Acid Orange 24	613/1975/T75
--	C.I. Disperse Brown 1	607/1975/Tp75
5850168	C.I. Acid Brown 14	538/1975/T75
3468631	C.I. Pigment Orange 5	523/1975/T75
2610119	C.I. Direct Red 81	518/1975/T75
--	C.I. Direct Yellow 84	504/1975/T75
91349	C.I. Direct Yellow 4	502/1975/T75
5610640	C.I. Acid Black 52	501/1975/Tp75 (sales)
3121742	C.I. Acid Black 1	427/1975/T75
6406560	C.I. Acid Red 151	418/1975/T75
4531491	C.I. Pigment Yellow 17	415/1975/T75
14097031	C.I. Basic Red 18	391/1975/T75
12225126	C.I. Pigment Yellow 73	389/1975/T75
6250233	C.I. Disperse Yellow 23	388/1975/T75
12210029	C.I. Acid Red 337	380/1975/T75
--	C.I. Disperse Orange 37	379/1974/T74

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
6505288	C.I. Pigment Orange 16	377/1975/T75
--	FD & C Red No. 40	364/1975/T75
10300740	C.I. Direct Brown 95	346/1975/T75
3351051	C.I. Acid Blue 113	340/1975/T75
2512290	C.I. Pigment Yellow 1	338/1975/T75
2610108	C.I. Direct Red 80	335/1975/T75
6420413	C.I. Direct Orange 102	332/1975/T75 (sales)
--	C.I. Direct Black 22	329/1975/T75
12222003	C.I. Direct Blue 80	306/1975/T75
12235222	C.I. Acid Yellow 159	291/1975/T75
4438168	C.I. Basic Orange 1	290/1974/T74
12220109	C.I. Acid Orange 116	279/1975/T75
1934210	C.I. Acid Yellow 23	271/1975/T75
--	C.I. Disperse Orange 29	271/1975/T75
495545	C.I. Basic Orange 2	265/1975/T75
--	C.I. Direct Yellow 44	262/1975/T75
6459945	C.I. Acid Red 114	258/1975/T75
2429734	C.I. Direct Blue 2	243/1975/T75 (sales)
--	C.I. Azoic Diazo Component 3, salt	241/1975/T75
2429745	C.I. Direct Blue 15	241/1974/T74
12223222	C.I. Disperse Orange 25	240/1975/T75
5102830	C.I. Pigment Yellow 13	240/1975/T75

Class: Azo Compounds

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
633965	C.I. Acid Orange 7	231/1975/T75
6471494	C.I. Pigment Red 23	228/1975/T75
--	C.I. Acid Orange 60	212/1975/T75
4482251	C.I. Basic Brown 4	212/1975/T75
3520727	C.I. Pigment Orange 13	209/1975/T75
1836222	C.I. Pigment Red 60	209/1975/T75
6486233	C.I. Pigment Yellow 3	192/1975/T75
--	C.I. Azoic Diazo Component 13, salt	191/1975/T75
--	C.I. Azoic Diazo Component 14, salt	184/1974/T74
104234	p-((p-Aminophenyl)azo)benzenesulfonic acid	178/1975/T75
12223380	C.I. Disperse Red 65	176/1975/T75
5850862	C.I. Acid Orange 8	175/1975/T75
1936158	C.I. Acid Orange 10	170/1975/T75
--	2,5-Diethoxy-4-morpholinobenzenediazonium chloride	170/1975/T75
1787617	C.I. Mordant Black 11	169/1975/T75
--	C.I. Disperse Red 177	167/1975/T75
3179893	C.I. Disperse Red 17	166/1975/T75
2610051	C.I. Direct Blue 1	157/1975/T75
--	C.I. Azoic Diazo Component 9, salt	155/1975/T75
3441143	C.I. Direct Red 23	155/1975/T75
6420446	C.I. Direct Red 24	152/1975/T75
2814779	C.I. Pigment Red 4	144/1975/T75
4335095	C.I. Direct Green 6	143/1974/T74

Class: Azo Compounds

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
12218961	C.I. Acid Black 107	138/1975/T75
12217377	C.I. Acid Red 266	138/1975/T75 (sales)
--	C.I. Direct Red 72	138/1975/T75
3626286	C.I. Direct Green 1	132/1975/T75
2429847	C.I. Direct Red 1	132/1975/T75
4477796	C.I. Solvent Red 26	128/1974/T74 (sales)
--	C.I. Azoic Diazo Component 12, salt	125/1975/T75
2429825	C.I. Direct Brown 2	125/1975/T75
16521349	C.I. Pigment Brown 5	123/1975/T75
--	p-Diethylaminobenzenediazonium chloride	122/1975/T75
--	C.I. Direct Blue 191	120/1974/T74 (sales)
1325548	C.I. Direct Orange 39	109/1975/T75
6656037	C.I. Direct Blue 98	107/1975/T75
12223200	C.I. Disperse Orange 17	107/1975/T75
6370087 (158:1)	C.I. Acid Blue 158, 158:1, 158:2	105/1975/T75
3791682	C.I. Acid Yellow 17	100/1975/T75
--	p-Dimethylaminobenzenediazo sodium sulfonate	100/1975/SRI (use)
15793734	C.I. Pigment Orange 34	99/1975/T75
--	C.I. Direct Blue 120 and 121A	97/1975/T75

Class: Azo Compounds

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod.(Thousand Pounds)/Year/Source
6227026	C.I. Direct Red 16	91/1974/T74 (sales)
6054484	C.I. Disperse Black 1	89/1974/T74
2872528	C.I. Disperse Red 1	89/1975/T75
5413752	C.I. Acid Red 73	87/1975/T75
8003223	C.I. Solvent Yellow 33	87/1975/T75
--	C.I. Direct Red 83	85/1975/T75
3761533	Acid Red 26	84/1975/T75
730405	C.I. Disperse Orange 3	81/1975/T75 (sales)
6655841	C.I. Pigment Red 17	81/1975/T75
12217640	C.I. Direct Orange 72	79/1975/T75
6420402	C.I. Direct Orange 29	76/1975/T75
60093	p-Phenylazoaniline (p-aminoazaobenzene) and hydrochloride	75/1975/T75 (sales)
587984	C.I. Acid Yellow 36	74/1975/T75
2429814	C.I. Direct Brown 31[1]	73/1975/T75
6410102	C.I. Pigment Red 2	73/1975/T75
6232560	C.I. Disperse Orange 5	72/1975/T75
3626402	C.I. Direct Blue 120	70/1975/T75
6448959	C.I. Pigment Red 22	68/1975/T75
3567655	C.I. Acid Red 85	67/1975/T75
3769571	C.I. Disperse Red 5	67/1975/T75

Class: Azo Compounds

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
12220643	C.I. Acid Yellow 19	65/1975/T75
3530196	C.I. Direct Red 37	63/1975/T75
6222635	C.I. Acid Red 137	62/1975/T75
5160021	D.&C. Red No. 9	62/1975/T75
6410419	C.I. Pigment Red 5	60/1975/T75
1937344	C.I. Direct Red 79	57/1974/T74 (sales)
6372969	C.I. Acid Yellow 40	56/1975/T75 (sales)
6439538	C.I. Disperse Yellow 5	56/1975/T75
992596	C.I. Direct Red 2	53/1975/T75
3626366	C.I. Direct Orange 26	52/1975/T75
2481949	C.I. Solvent Yellow 56	50/1975/T75
8006051	C.I. Direct Blue 126	49/1974/T74
3564270	C.I. Mordant Orange 6	49/1975/T75
12222376	C.I. Direct Orange 34	47/1975/T75
3687807	C.I. Direct Red 26	47/1975/T75 (sales)
3701404	C.I. Acid Red 99	45/1975/T75 (sales)
16143796	C.I. Direct Blue 76	44/1975/T75
6406322	C.I. Acid Blue 118	43/1975/Tp75 (sales)
6358298	C.I. Direct Red 39	43/1975/T75
21416466	C.I. Pigment Red 63	43/1975/T75

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
5858399	C.I. Acid Red 4	39/1975/T75
5850395	C.I. Acid Green 20	38/1975/T75
--	C.I. Acid Red 182	38/1975/T75
2150541	C.I. Direct Blue 25	36/1975/T75 (sales)
--	C.I. Azoic Diazo Component 8, salt	35/1975/T75
2429790	C.I. Direct Orange 8	35/1975/T75 (sales)
10343585	C.I. Acid Yellow 99	34/1975/T75 (sales)
6420413	C.I. Direct Red 4	34/1974/T74
6410135	C.I. Pigment Red 6	34/1975/T75
--	C.I. Azoic Diazo Component 10, salt	33/1974/T74 (sales)
3618620	C.I. Mordant Brown 33	33/1974/T74 (sales)
2870328	C.I. Direct Yellow 12	32/1975/T75
--	C.I. Azoic Diazo Component 1, salt	30/1975/T75 (sales)
2429712	C.I. Direct Blue 8	30/1975/T75
3861732	C.I. Acid Blue 92	29/1975/T75 (sales)
1681603	C.I. Acid Violet 3	29/1975/T75 (sales)
12221873	C.I. Direct Black 9	29/1975/Tp75 (sales)

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
6226808	C.I. Acid Red 115	28/1974/T74 (sales)
--	C.I. Pigment Violet 3	28/1975/T75 (sales)
6656037	C.I. Direct Yellow 28	27/1975/T75
6375559	C.I. Acid Yellow 42	26/1975/T75
--	C.I. Azoic Diazo Component 5, salt	25/1975/T75
--	C.I. Acid Orange 64	24/1975/T75 (sales)
6391215	C.I. Direct Orange 73	23/1975/T75
--	D.&C. Red No. 6	22/1975/T75
10127272	C.I. Acid Orange 74	20/1975/T75
6408908	C.I. Acid Yellow 65	20/1975/T75 (sales)
1052386	C.I. Basic Brown 1	20/1975/T75
--	C.I. Solvent Brown 12	20/1974/T74
--	D.&C. Red No. 7	20/1975/T75
2611827	C.I. Acid Red 18	19/1975/T75 (sales)
--	C.I. Azoic Diazo Component 49, salt	19/1975/T75 (sales)
6360072	C.I. Acid Red 37	18/1975/T75
--	C.I. Acid Yellow 38	18/1975/T75 (sales)
13195192	C.I. Acid Yellow 54	17/1975/T75 (sales)

Class: Azo Compounds

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
3564156	C.I. Mordant Brown 1	16/1974/T74 (sales)
3618631	C.I. Mordant Red 7	15/1975/T75 (sales)
--	p-(Ethyl(2-hydroxyethyl)amino)benzenediazonium chloride	15/1975/T75
12223357	C.I. Disperse Red 50	14/1975/T75
1658566	C.I. Acid Red 88	13/1975/T75 (sales)
2503733	C.I. Direct Blue 78	13/1975/T75 (sales)
97563	4-(o-Tolylazo)-o-toluidine (o-Aminoazotoluene)	12/1975/T75 (sales)
6359826	C.I. Acid Yellow 11	11/1975/T75
2429836	C.I. Direct Black 4	11/1974/T74 (sales)
60117	C.I. Solvent Yellow 2 (p-Dimethylaminoazobenzene)	11/1974/T74 (sales)
6625463	C.I. Acid Violet 12	10/1975/T75 (sales)
6359906	C.I. Acid Yellow 34	10/1975/T75 (sales)
--	D.&C. Red No. 34	9/1974/T74
12236736	C.I. Pigment Yellow 83	9/1974/T74 (sales)
4321691	C.I. Acid Violet 7	8/1975/T75 (sales)

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS (continued)

CAS No.	Chemical Name	Annual Prod. (Thousand Pounds)/Year/Source
1325617	C.I. Direct Orange 37	8/1975/T75 (sales)
--	C.I. Acid Red 186	7/1975/T75 (sales)
6472500	C.I. Acid Red 89	6/1975/Tp75 (sales)
10130297	C.I. Direct Yellow 8	6/1975/T75 (sales)
--	D.&C. Red No. 12	5/1975/T75
6441914	C.I. Acid Violet 1	4/1975/T75 (sales)
--	D.&C. Red No. 36	4/1975/T75 (sales)
2829438	C.I. Direct Red 75	3/1975/T75 (sales)

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[1] Data includes dyes which are similar to, but not chemically identical with the indicated C.I. name.

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE[†]

CAS No.	Chemical Name
120683	m-(4-Amino-3-tolylazo)benzenesulfonic acid
133608	Azosulfamide
136403	Phenazopyridine hydrochloride
144752	Sodium sulfoxone
599791	Sulfasalazine (salicylazosulfapyridine)
4080313	1-(3-Chloroallyl)-3,5,7-triazo-1-azoniaadamantane chloride
--	5-Amino-4,5'-dihydroxy-3,4'-((2-methoxy-5-methyl-p-phenylene)bis(azo))-di-2,7-naphthalenedisulfonic acid,5'-benzenesulfonate
--	2-(2-Amino-5-hydroxy-7-sulfo-1-naphthylazo)-5-nitrobenzoic acid
--	m-((4-Amino-3-methoxyphenyl)azo)benzenesulfonic acid
--	4-((4-Amino-5-methoxy-o-tolyl)azo)-4-hydroxy-2,7-naphthalenedisulfonic acid, benzenesulfonate
--	3-(4-Amino-5-methoxy-o-tolylazo)-1, 5-naphthalenedisulfonic acid
--	7-((4-Amino-5-methoxy-o-tolyl)azo)-1,3-naphthalenedisulfonic acid
--	2-(2-Amino-1-naphthylazo-4-(1,1,3,3-tetramethylbutyl)phenol
--	m-((p-Aminophenyl)azo)benzenesulfonic acid
--	7-((4-Aminophenyl)azo)-1,3-naphthalenedisulfonic acid
--	5-Amino-8-(phenylazo)-2-naphthol
--	8-Amino-5-(phenylazo)-2-naphthol
--	5-((p-Aminophenyl)azo)salicylic acid
--	3-((4-Amino-o-tolyl)azo)-1,5-naphthalenedisulfonic acid
--	7-((4-Amino-o-tolyl)azo)-1,3-naphthalenedisulfonic acid
--	4',4'''-Azobis(4-biphenylcarboxylic acid)
--	5-(Bis(2-hydroxyethyl)amino)-2,2'-chloro-4-nitrophenylazobenzanilide
--	2,4-Bis(xylazo)resorcinol

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE† (continued)

CAS No.	Chemical Name
--	3-Chloro-4-diethylaminobenzenediazonium chloride(p-diazo-2-chloro-N,N-diethylaniline)-zinc chloride
--	N-((5-Chloro-o-tolyl)azo)sarcosine
--	1,4-Diazobicyclo(2.2.2)octane
--	4-Diazo-2,4-diethoxy-1-thio-p-cresylbenzene zinc salt
--	Diazodinitrophenol
--	4-Diazo-1-morpholine benzene zinc chloride
--	α-Diazo-1-naphthol-5-sulfonate
--	2-Diazo-1-naphthol-5-sulfonic acid, sodium salt
--	Dibenzylazodicarboxylate
--	3-((4'-N,N-Diethylamino)phenylazo)-1H-1,2,4-triazole
--	N',N'-((3,3'-Dimethoxy-4,4'-biphenylylene)bis(azo))bis (N-methyltaurine)
--	1-(3,5-Dinitro-2-hydroxyphenylazo)-2-hydroxynaphthalene
--	2-(N-Ethyl-p-((6-methoxy-2-benzothiazolyl)azo)anilino)-ethanol
--	N-(7-Hydroxy-8-((2-hydroxy-5-nitrophenyl)azo)-1-naphthyl)acetamide
--	7-Hydroxy-8-((4'-((p-hydroxyphenyl)azo)-3,3'-dimethyl-4-biphenylyl)azo)-1,3-naphthalenedisulfonic acid
--	4'-Nitro-4-amino-3-methoxyazobenzene
--	2-(o-Nitrophenylazo)-p-cresol (CH_2=1)
--	2-o-Nitrophenylazo)-4,1-ditertamylphenol (OH=1)
--	4-(Phenylazo)diphenylamine
--	4-(2,5-Xylylazo)-o-toluidine

AZO COMPOUNDS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS FOR WHICH EXACT FIGURES ARE NOT AVAILABLE[†] (continued)

[†] Compiled from Synthetic Organic Chemicals, United States Production and Sales, 1975, excluding the Dyes and Pigments sections. Because of the large number of chemicals listed in these sections on dyes and pigments for which exact structures would have to be determined, these have not been included in this table. Chemicals from the section on medicinals were included only if an initial examination of the names listed indicated that they fit the category. CAS Numbers were included only if found in one search of readily available sources.

9. Class IX: Nitrofurans

These compounds are noted for their antimicrobial activity, and their only uses have been in drug-related applications. They have been used as prophylactic additives and growth promoters in feeds for poultry and swine, in treatment of genitourinary, gastrointestinal, and surface infections in humans and domestic animals, and in treatment of mammary gland infections in dairy cattle. The accompanying tables summarize the available information on production of nitrofurans. Of the more than 2000 nitrofurans reported in the literature, only those nitrofurans presently in commercial production or those for which there is some indication of past commercial production are listed.

Class: Nitrofurans

NITROFURANS WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
59870	5-Nitro-2-furaldehyde semicarbazone (Nitrofurazone)	>1000 lbs./1975/T75
67209	Nitrofurantoin	>1000 lbs./1975/T75
67287	Nihydrazone	>1000 lbs./1977/SRI
67458	Furazolidone	>1000 lbs./1975/T75
92557	5-Nitro-2-furanmethanediol, diacetate	>1000 lbs./1975/T75
3270711	Nifuraldezone	>1000 lbs./1977/SRI

Class: Nitrofurans

NITROFURANS WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
139913	Furaltadone
531828	N-(4-(5-Nitro-2-furyl)-2-thiazolyl)acetamide
555840	1-((5-Nitrofurfurylidene)amino)-2-imidazolidinone
586845	5-Nitro-2-furfurylmethyl ether
609392	Nitrofuran
712685	2-Amino-5-(5-nitro-2-furyl)-1,3,4-thiadiazole (Triafur)
946485	Guanofuracin
1614206	Nifurprazine
3570750	2-(2-Formylhydrazino)-4-(5-nitro-2-furyl)thiazole
6236051	Nifuroxime
24554265	N-(4-(5-Nitro-2-furyl)-2-thiazolyl)formamide
25962770	trans-2-((Dimethylamino)methylimino)-5-(2-(5-nitro-2-furyl)vinyl)-1,3,4-oxadiazole

10. Class X: Azides

This small group of compounds has no chemicals with an annual production greater than one million pounds. Most of these compounds are specialty reagents or experimental chemicals. Sodium and potassium azides have been experimentally tested as herbicides, and sodium azide has been suggested as the detonating agent for inflatable air bags in automobiles. Lead azide has been used in commercial blasting caps and in military ammunition, but no data were found on the volume of production, since it is presumably produced by the military.

Class: Azides

AZIDES WITH ANNUAL PRODUCTION GREATER THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name	Annual Prod./Year/Source
1070195	Carbonazidic acid, 1,1-dimethylethyl ester (tert-butyl carbazate)	>1000 lbs./1977/SRI
14546442	Hydrazine azide	>1000 lbs./1977/SRI
18810587	Barium azide	>1000 lbs./1977/SRI
22750578	Cesium azide	>1000 lbs./1977/SRI
23325911	2,6-Bis(p-azidobenzylidene)-4-methylcyclohexanone	>1000 lbs./1975/T75

Class: Azides

AZIDES WITH ANNUAL PRODUCTION LESS THAN ONE THOUSAND POUNDS

CAS No.	Chemical Name
13424469	Lead azide
13838089	Azidoamphenicol (Leukomycin)
17243388	Azidocillin (α-azidobenzylpenicillin)
26628228	Sodium azide
--	Potassium azide
--	Silver azide

V. STUDY OF POTENTIAL CARCINOGENICITY OF SELECTED CHEMICALS BASED ON STRUCTURE-ACTIVITY ANALYSIS

The purpose of this study was to provide qualitative methods for identifying those substances within specific chemical classes with the greatest potential for carcinogenicity on the basis of their structural features. The Project Officer selected three classes for this initial study: epoxides, alkyl halides, and vinyl halides.

For each of these classes, the Project Officer provided a list of chemicals known to be commercially significant (i.e., found in the Directory of Chemical Producers-U.S.A., 1971), and SRI supplemented the lists with other chemicals judged to have significant human exposure (e.g., chemicals identified by the EPA in drinking water supplies).

As a first step in the analysis, published animal carcinogenicity data on the three classes were compiled and evaluated. All chemicals belonging to these classes were considered, not just those on the list described above (i.e., commercially significant or judged to have human exposure). Next, the data for chemicals in each class were studied. Structural features common to the carcinogens were identified as well as those common to the inactive chemicals. Criteria were then developed for estimating the potential carcinogenicity of chemicals in each class on the basis of these significant structural features. Where possible, the criteria were supported by reference to publications by carcinogenesis experts.

After the criteria were defined, they were applied to estimating the potential carcinogenicity of the commercially significant and other chemicals known to have human exposure, but for which animal carcinogenicity data were not available. For those chemicals on the lists of those to be analyzed for which there were animal test data, the estimate of potential carcinogenicity was based on the results of the tests rather than on the structural criteria alone. For each chemical class studied, a report was prepared consisting of two parts: (1) a discussion of the structural criteria used in estimating potential carcinogenicity, and (2) a table containing the names, CAS numbers, and structures of the chemicals analyzed, and an estimate of potential carcinogenicity for each chemical--made either on the basis of the structural criteria or existing animal test data. These three reports are presented on pages 5-3 through 5-86.

A. Epoxides

All aliphatic monoepoxides in which the epoxide is terminal are judged to be suspect. Although the carcinogenicity of short chain monoepoxides, such as ethylene oxide, has not been demonstrated adequately, some of these chemicals have been shown to alkylate DNA. On the basis of available carcinogenicity data, monoepoxides with longer aliphatic chains (i.e., those which are more hydrophobic) are considered to be of higher suspicion than the short chain chemicals. The presence of a double bond, aldehyde (as in glycidaldehyde), or other potentially reactive functional groups near the epoxide also increases the suspicion by raising the possibility that the chemical can act as a difunctional alkylating agent for DNA. In addition, chemicals which are readily metabolized to aliphatic monoepoxides (e.g., by ester hydrolysis) are also considered suspect.

On the basis of available carcinogenesis data:

(a) Cyclic aliphatic monoepoxides and compounds readily metabolized to cyclic aliphatic monoepoxides are not considered suspect.

(b) Diepoxides are considered to be highly suspect, excepting those which are potentially sterically hindered from acting as difunctional crosslinking agents for DNA. Van Duuren (Ann. N.Y. Acad. Sci. 163, 633-651, 1969) has suggested that the diepoxides may be inactive as carcinogens if the maximal atomic distance between the epoxides is <4.0Å or >9.9Å based on Dreiding scale models.

(c) Aliphatic chemicals which have single epoxides embedded in the chain or in which one of the carbons contained in the epoxide ring(s) is fully substituted are not considered suspect.

Compounds in which cleavage of the epoxide may lead to resonance stabilized carbonium ions (e.g., styrene oxide) are considered suspect.

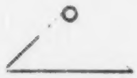
EPOXIDES

*Potential Carcinogenicity

ETHYLENE OXIDE
CAS NO. = 75-21-8

C

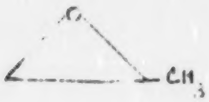
(Test data reported, but inadequate for evaluation; see Lawley, 1976[1] and IARC 11, 157, 1976[2])



PROPYLENE OXIDE
CAS No. = 75-56-9

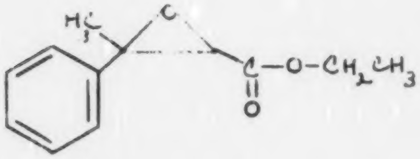
C

(Positive test results reported; see Lawley, 1976[1])



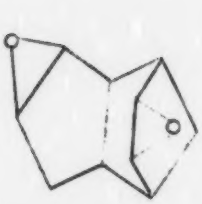
OXIRANE CARBOXYLIC ACID, 3 METHYL -3 PHENYL-, ETHYL ESTER
CAS No. = 77-83-8

C



DICYCLOPENTADIENE DIEPOXIDE
CAS No. = 81-21-0

C



1. Lawley, P.D., "Carcinogenesis by Alkylating Agents" in Searle, C.E., ed., Chemical Carcinogens, ACS Monograph 173, American Chemical Society, Washington, D.C., 1976, pp. 83-244.

2. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Man, Vol. 11, International Agency for Research on Cancer, Lyon, 1976, pp.125-159.

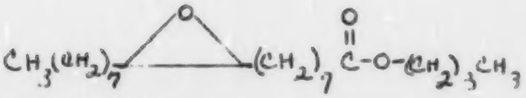
EPOXIDES (continued)

*Potential Carcinogenicity

9, 10-EPOXYSTEARIC ACID, BUTYL ESTER
CAS No. = 106-83-2

N

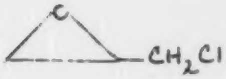
(Negative test results reported; see Lawley, 1976)



EPICHLOROHYDRIN
CAS No. = 106-89-8

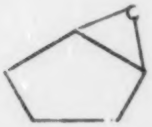
C

(Positive test results reported; see Lawley, 1976)



EPOXYCYCLOPENTANE
CAS No. = 285-67-6

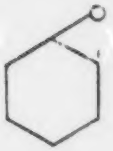
N



EPOXYCYCLOHEXANE
CAS No. = 286-20-4

N

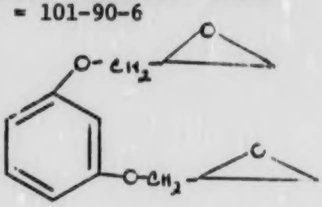
(Negative test results reported; see Lawley, 1976)



EPOXIDES (continued)

*Potential Carcinogenicity

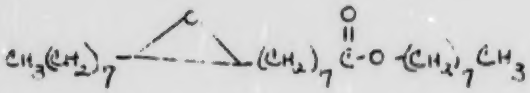
RESORCINOL, DIGLYCIDYL ETHER
CAS No. = 101-90-6



C

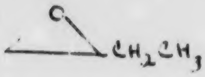
(Test data reported, but inadequate for evaluation; see Lawley, 1976, and IARC 11, 125, 1976)

9, 10-EPOXYSTEARIC ACID, OCTYL ESTER
CAS No. = 106-84-3



N

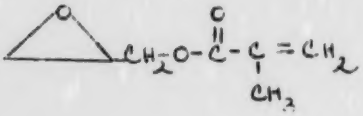
OXIRANE, ETHYL
CAS No. = 106-88-7



C

(Positive test results reported; see Lawley, 1976)

2-PROPENOIC ACID, 2-METHYL-, GLYCIDYL ESTER
CAS No. = 106-91-2



C

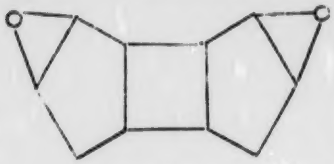
EPOXIDES (continued)

*Potential Carcinogenicity

CYCLOBUTA (1", 2":3, 4; 4", 3":3' 4')

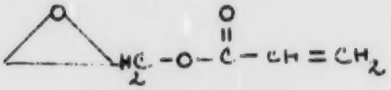
DICYCLOPENTA (1, 2-b:1', 2'-b')
BISOXIRENE, DECAHYDRO
CAS No. = 7163-39-5

C



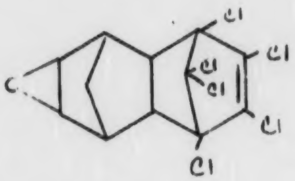
ACRYLIC ACID, GLYCIDYL ESTER
CAS No. = 106-90-1

C


O
O
H2C -O- C - CH = CH2

DIELDRIN
CAS No. = 60-57-1

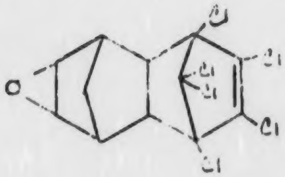
(CLASSIFY AS HALIDE)


Cl
Cl
Cl
Cl
Cl
Cl

endo, exo

ENDRIN
CAS No. = 72-20-8

"


O
Cl
Cl
Cl
Cl
Cl
Cl

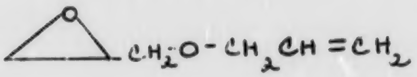
endo, endo

EPOXIDES (continued)

*Potential Carcinogenicity

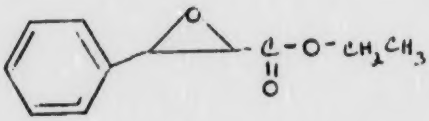
2-PROPENE GLYCIDYL ETHER
CAS No. = 106-92-3

C


O
CH₂-O-CH₂CH=CH₂

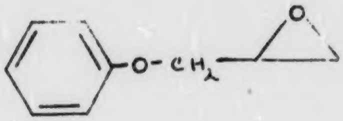
OXIRANE CARBOXYLIC ACID, 3-PHENYL-, ETHYL ESTER
CAS No. = 121-39-1

C


O
C-O-CH₂CH₃
O

OXIRANE, PHENOXYMETHYL
CAS No. = 122-60-1

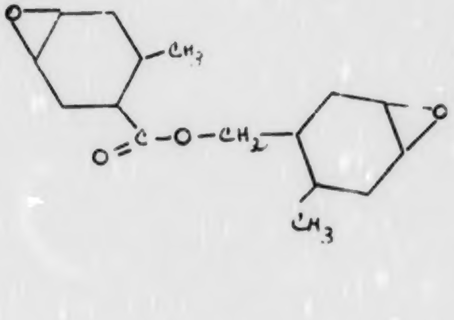
C



3,4-EPOXY-6-METHYL-CYCLOHEXYLMETHYL 3,4-EPOXY-6-METHYL-CYCLOHEXANE CARBOXYLATE
CAS No. = 141-37-7

C

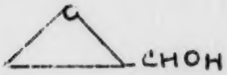
(Positive test results reported; see Lawley, 1976)


O
CH₃
O=C-O-CH₂
O
CH₃

EPOXIDES (continued)

*Potential Carcinogenicity

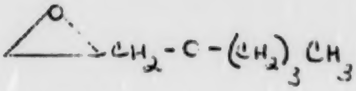
GLYCIDOL
CAS No. = 556-52-5



C

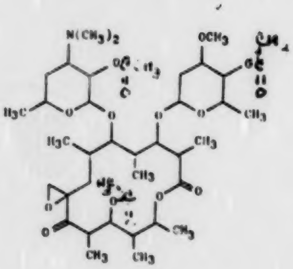
(Test results reported but inadequate for evaluation; see Lawley, 1976)

BUTYL GLYCIDYL ETHER
CAS No. = 556-52-5


O
CH2-C-(CH2)3CH3

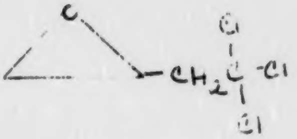
C

OLEANDOMYCIN TRIACETATE
CAS No. = 2751-09-9



N

OXIRANE, (2,2,2-TRICHLOROETHYL)
CAS No. = 3083-25-8


O
CH2C-Cl
Cl
Cl

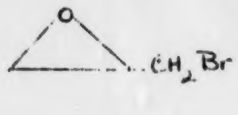
C

EPOXIDES (continued)

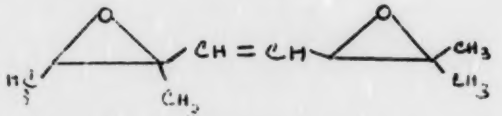
*Potential Carcinogenicity

EPIBROMOHYDRIN C
CAS No. = 3132-64-7

(Test results reported
but inadequate for evaluation;
see Lawley, 1976)

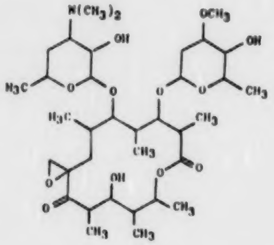


OXIRANE, 2-(2-(3,3-DIMETHYLOXIRANYL)ETHENYL)-2,3-DIMETHYL C
CAS No. = 3765-28-4



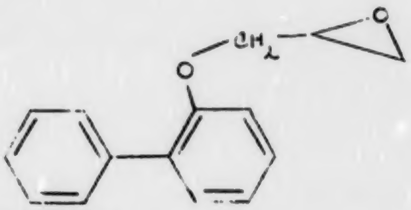
O
CH = CH
O
CH3
CH3
CH3

OLEANDOMYCIN N
CAS No. = 3922-90-5



N(CH3)2
OH
OCH3
OH
H3C
CH3
O
H3C
CH3
CH3
OH
O
CH3
CH3
CH3

OXIRANE, (((1,1'-BIPHENYL)-2-YLOXY)METHYL) C
CAS No. = 7144-65-2



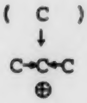
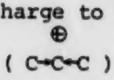
---

* C = suspect as potential carcinogen
N = not suspect as potential carcinogen

B. Alkyl Halides

Increasing potential to form a stable carbonium ion was used as the primary criterion of increasing alkylating ability, and, hence, of increasing suspected carcinogenicity for alkyl halides. The estimate of potential to form a stable carbonium ion was based on structural and chemical properties as follows:

(1) Strength of the R-X bond. For example, the electronegativity of fluorine is so large, and its bond to carbon is so strong, that most alkyl fluorides would be expected to be inactive. Among analogous compounds, chlorides would be expected to be less reactive than bromides, which would be less reactive than iodides (e.g., Morrison and Boyd, 1973, pp. 479-480).

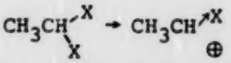
(2) Electronic effects of nearby substituents and bonds (electron-donating or electron-withdrawing groups, and resonance bonds). Among aliphatic halides, the electron-donating effect of alkyl groups alone is an important factor. Thus tertiary carbonium ions are very stable since the three groups each donate some electronic charge to the positively charged carbon ( $\begin{array}{c}C\\ \downarrow\\ C\rightarrow C\leftarrow C\\ \oplus\end{array}$). Secondary carbonium ions ( $\overset{\oplus}{C\rightarrow C\leftarrow C}$) are less stable since only two groups are donating electrons, and similarly, primary carbonium ions ($C\rightarrow C\ \oplus$) are the least stable of the three (Morrison and Boyd, 1973, p. 164).

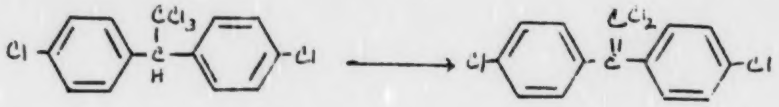
Increased chain length would be expected to enhance carbonium ion stability among analogous compounds. Inductive effects may be felt through up to four carbon atoms, so that loss of a bromide ion from 2-bromohexane would yield a more stable carbonium ion than that of 2-bromopropane

(Morrison and Boyd, 1973, p. 600). In chains longer than four carbon atoms, it is difficult to predict electronic effects of atoms distal to the halide.

An additional factor which may be considered in the prediction of carbonium ion stability is rearrangement, such as a hydride or alkyl shift. For example, upon loss of the bromide ion from n-bromopentane, the primary carbonium ion may rearrange to a secondary one via a hydride shift (Morrison and Boyd, 1973, pp. 171-172).

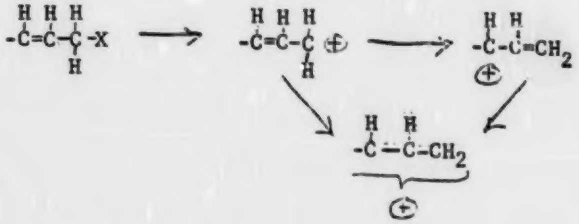
Nearby electron-donating or electron-withdrawing groups may also be expected to stabilize or destabilize the carbonium ion, respectively. For example, in addition to alkyl groups, amine and hydroxyl groups stabilize positive charge. Therefore, the secondary cation of n-propyl alcohol would be more stable than the isopropyl carbonium ion. In contrast, aldehydes, ketones, and carboxylic acid groups withdraw electrons, so that the α-carbonium ion of propionaldehyde would be less stable than the isopropyl cation. The halides are also strong electron-withdrawing groups, the strength (electronegativity) decreasing in the series from fluoride to iodide (Morrison and Boyd, 1973, p. 360).

Compounds which, by their activity, demonstrate an exception to this concept are gem-substituted halides. It would be expected that a carbonium ion formed from such a compound would be destabilized by the electron-withdrawing halide remaining ( $\mathrm{CH_3CH}\genfrac{}{}{0pt}{}{X}{X} \rightarrow \mathrm{CH_3CH}\genfrac{}{}{0pt}{}{X}{\oplus}$). However, several gem-substituted halides have been implicated as carcinogens in animal tests (CCl_4,$CHCl_3$, DDT). A possible mechanism for activation would be metabolic dehydrohalogenation to yield vinyl halide derivatives, since this reaction is known to occur in DDT (IARC, 5, 102):



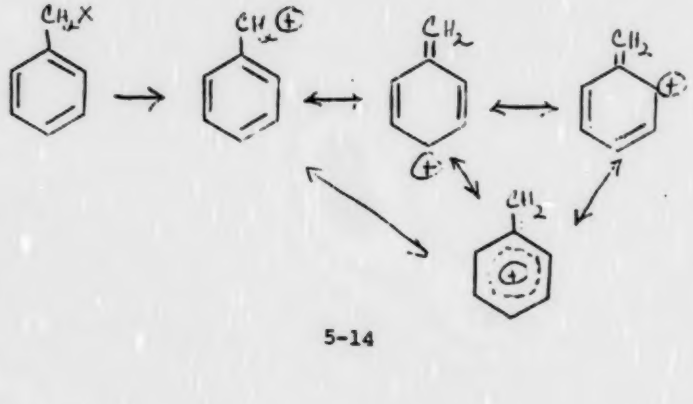
These vinyl derivatives may then be activated to potent alkylating agents via epoxidation (Weisburger and Williams, 1975).

Alkyl halides would be expected to yield extremely stable carbonium ions because of the resulting resonance and delocalization of charge over three carbon atoms:

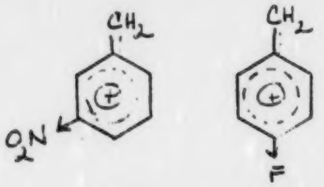


Included in the aliphatic group are organophosphates which contain aliphatic halide fragments, since hydrolysis can readily free these fragments to act as alkylating agents in the usual way.

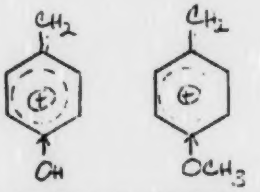
A benzyl halide may lose a halide to yield the benzyl carbonium ion, which is stabilized by the delocalization of electrons in the benzene ring:



(Morrison and Boyd, 1973, pp. 397-398). The degree of stabilization appears to depend to some extent upon the presence or absence of electron-withdrawing or donating groups on the ring:



destabilized slightly more
than the benzyl cation



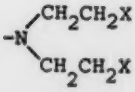
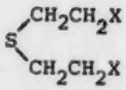
stabilized slightly more
than the benzyl cation

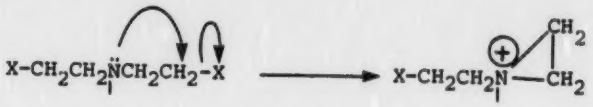
Electron-withdrawing groups usurp a portion of the electronic charge which would otherwise help delocalize the positive charge, while electron-donating groups contribute additional electronic charge.

Polycyclic aromatic alkyl halides similarly contain a high degree of delocalization of electrons, which greatly stabilizes the carbonium ion. However, another significant factor in the carcinogenicity of these chemicals may be their ability to intercalate between the DNA strands (Searle, 1976, pp. 280-281).

In addition to the considerations above, potential activity was predicted on the basis of structural relationship to known carcinogens or potent alkylating agents as was described above for gem-halides. Some other examples follow:

(1) Halogenated ethers could be ranked with the corresponding non-ether aliphatic halides containing electron-donating groups (RO-). However, these compounds are more highly suspect because of the known carcinogenicity of several haloethers (bis(chloromethyl)ether and chloromethyl methyl ether; see IARC, 4, 231, and Nelson, 1973).

(2) Mustards ( $-N(CH_2CH_2X)_2$ or  $S(CH_2CH_2X)_2$) are believed to yield stable cations, upon loss of a halogen ion, as a result of the formation of a cyclic immonium ion:



The immonium or sulfonium ion may then react with the nucleophilic centers in the bases of DNA (Price, et al., 1969). It has been suggested that mustards, which are difunctional, are particularly effective as alkylating agents because of their ability to form cross-linkages in the DNA or between DNA and protein (Searle, 1976, p. 206). Half-mustards ($>N-CH_2CH_2X$ or $-S-CH_2CH_2X$) can also alkylate DNA, but are not capable of forming the same types of cross-linkages.

(3) Subsitituted methane compounds (except for fluorinated compounds) are in general suspect of having carcinogenic activity based on the known carcinogenicity of chloroform and carbon tetrachloride.

(4) Alkyl halide esters of phosphoric acid are considered suspect on the basis of the recently reported carcinogenicity of Tris-BP.

It should also be noted that for some classes of halides (e.g., Freons) there was neither clearcut experimental evidence nor a compelling structure-activity analogy to use in estimating potential carcinogenicity. Such chemicals were designated as unknown.

References

Morrison, R. T. and Boyd, R. N., Organic Chemistry, Third Edition, Allyn and Bacon, Inc., Boston, Massachusetts, 1973, pp. 479-480

Weisburger, J. H. and Williams, G. M., Metabolism of Chemical Carcinogens. In: Becker, F. F. (ed.), Cancer, A Comprehensive Treatise, Plenum Press, New York and London, 1975, p. 185

Searle, C. E. (ed.), Chemical Carcinogens, ACS Monograph 173, American Chemical Society, Washington, D.C., 1976

Price, et al., Ann. N. Y. Acad. Sci., 163(2), 1969, 591-598

IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Man, Vols 4 & 5, World Health Organization, International Agency for Research on Cancer, Lyon, France, 1974

Nelson, N., New England Journal of Medicine, 288(21), 1123-4, 1973

Key to Interpretation of Alkyl Halides Tables

Structure Class:

A	Aliphatic Monosubstituted	(C_1-C_4)	
B	Aliphatic Monosubstituted	(>C_4)	
C	Aliphatic Gem substituted	(C_1-C_4)	when compounds contains both gem and monosubstitution, gem takes precedence
D	Aliphatic Gem substituted	(>C_4)	
E	Cyclic		
F	Monosubstituted benzyl halides		
G	Gem-substituted benzyl halides		
H	Mustards (sulfur and nitrogen mustards)		
I	Polycyclic aromatic alkyl halides		

Groups A, C include compounds which can be easily broken down into C_1-C_4 fragments (e.g., butyl phosphates which are readily hydrolyzed to yield butyl alcohols).

Clarification of other structural characteristics in the molecule:

(1) Base analog

(2) "Symmetrical alkyl halides" which may be di- or tri-functional

The following are all classifications for difunctional compounds in which the second group is different and may also be active:

(3) halide + epoxide

(4) halide + potential intercalating structure

(5) halide + vinyl halide

(6) halide + acetylating group

(7) halide + other potentially active groups (e.g., nitroso, azo, nitro)

(1) Carcinogenicity

C = Substantial human or animal experimental evidence

C? = Limited evidence

N = Negative in a reliable test

+ = For S/A reasons limited suspicion of carcinogenicity

++ = For S/A reasons strong suspicion of carcinogenicity, e.g., possibility of forming resonance-stabilized carbonium ion

0 = no adequate experimental evidence and no compelling S/A analogy on which to base evaluation

(2) DCP-Darr - cited on list obtained by Darr from search of SRI-DCP data base

(3) Fishbein - cited on original list of chemicals from Fishbein

(4) EPA-H_2O - Organic Compounds Identified in Drinking Water in the United States, Health Effects Research Laboratory, EPA, Cincinnati, Ohio, July 1, 1976

(5) NCI - cited in tabulation of chlorides prepared for NCI-CSWG by Helmes and Poirier

C = on list of alkyl halides for which there is information on carcinogenicity

E = on list of halides with significant exposure

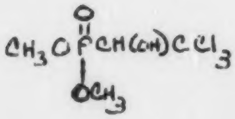
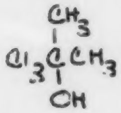
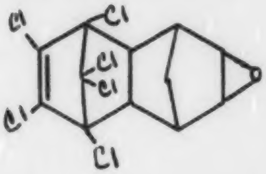
(6) Other

ACS = American Chemical Society Monograph - Chemical Carcinogenesis, 1976, followed by page number

IARC = International Agency for Research on Cancer Monograph Series, followed by volume number and page number

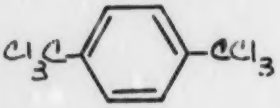
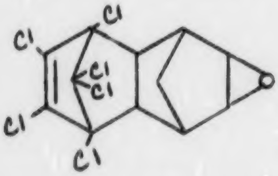
ALKYL HALIDES

I. CHLORIDES

Structure Class		(1) Carcinogenicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H$_2$O	(5) NCI(E/C)	(6) Other
C	(2,2,2-Trichloro-1-hydroxyethyl)-phosphonic acid, dimethyl ester CAS No.: 52-68-6  $CH_3O\overset{\overset{O}{\Vert}}{\underset{\underset{OCH_3}{\vert}}{P}}CH(OH)CCl_3$	C?	✓			✓ (C)	ACS, p. 170
C	Carbon tetrachloride CAS No.: 56-23-5 CCl_4	C	✓	✓	✓	✓ (E/C)	IARC, 1, 53; ACS, p. 158
C	2-Propanol, 1,1,1-trichloro-2 methyl- CAS No.: 57-15-8  $Cl_3\overset{\overset{CH_3}{\vert}}{\underset{\underset{OH}{\vert}}{C}}CH_3$	++	✓			✓ (E)	
E (3,5)	Dieldrin CAS No.: 60-57-1 	C	✓		✓	✓ (E/C)	IARC, 5, 125; ACS, p. 177

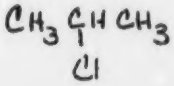
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
C	Chloroform CAS No.: 67-66-3 $HCCl_3$	C	✓	✓	✓	✓ (E/C)	IARC, 1, 61; ACS, p. 158
C	Hexachloroethane CAS No.: 67-72-1 Cl_3CCCl_3	+	✓				
G (2)	2,2-Hexachloroparaxylene CAS No.: 68-36-0 	++	✓				
C	Methyl chloroform CAS No.: 71-55-6 CH_3CCl_3	++	✓			✓ (E)	
E (3,5)	Endrin CAS No.: 72-20-8 	++	✓		✓	✓ (E)	IARC, 5, 157; ACS, p. 177

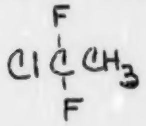
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
A	Chloromethane CAS No.: 74-87-3 CH_3Cl	++	✓	✓	✓	✓ (E)	
C	Bromochloromethane CAS No.: 74-97-5 $ClCH_2Br$	++	✓				
A	Alkylating agents, e.g., ethyl chloride CAS No.: 75-00-3 CH_3CH_2Cl	+			✓	✓ (E)	
C	Methylene chloride CAS No.: 75-09-2 H_2CCl_2	+	✓		✓	✓ (E)	ACS, p. 158
A	2-Chloropropane CAS No.: 75-29-6  $CH_3\underset{Cl}{\underset{\vert}{C}}HCH_3$	+	✓				

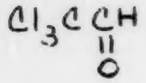
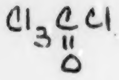
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
C	Dichlorofluoromethane CAS No.: 75-43-4 Cl_2CHF	+	✓				
C	Chlorodifluoromethane (Freon 22) CAS No.: 75-45-6 F_2CHCl	0	✓			✓ (E)	
C	Bromotrichloromethane CAS No.: 75-62-7 $BrCCl_3$	+	✓				
C	1-Chloro-1,1-difluoroethane CAS No.: 75-68-3  $ClCF_2CH_3$	0	✓			✓ (E)	
C	Trichlorofluoromethane CAS No.: 75-69-4 Cl_3CF	+	✓		✓	✓ (E)	

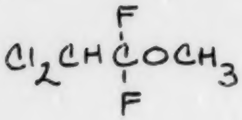
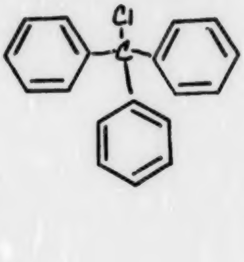
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
C	Dichlorodifluoromethane CAS No.: 75-71-8 Cl_2CF_2	0	✓			✓ (E)	
C	Aerosol propellants (e.g., Freon) CAS No.: 75-72-9 $ClCF_3$	0	✓				
C	1,2-Dibromo-1,1-dichloroethane CAS No.: 75-81-0 $BrCl_2CCH_2Br$	+	✓				
C (6)	Chloral (Trichloroacetaldehyde) CAS No.: 75-87-6  $Cl_3C\underset{\overset{\|}{O}}{C}H$	+	✓				
C (6)	Trichloroacetyl chloride CAS No.: 76-02-8  $Cl_3\underset{\overset{\|}{O}}{C}Cl$	+	✓				

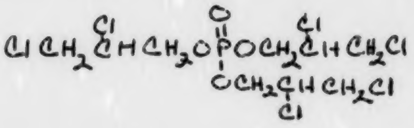
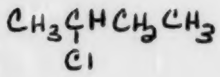
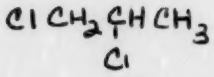
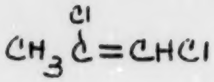
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
C	1,1,2,2-Tetrachloro-1,2-difluoroethane (Freon 112) CAS No.: 76-12-0 $Cl_2FCCFCl_2$	+	✓			✓ (C)	ACS p. 158
C	1,2-Dichloro-1,1,2,2-tetrafluoroethane (Freon 114) CAS No.: 76-14-2 ClF_2CCF_2Cl	0	✓			✓ (E)	
C	Chloropentafluoroethane CAS No.: 76-15-3 ClF_2CCF_3	0	✓			✓ (E)	
C	2,2-Dichloro-1,1-difluoroethyl methyl ether CAS No.: 76-38-0  $Cl_2CHCF_2OCH_3$	+	✓			✓ (E)	
F	Chlorotriphenyl methane CAS No.: 76-83-5 	++	✓				

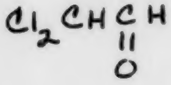
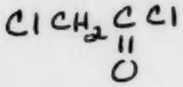
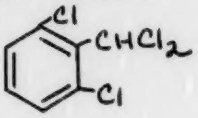
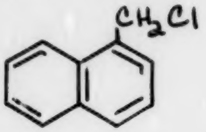
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
A	2,3-Dichloro-1-propanol, phosphate CAS No.: 78-43-3  $ClCH_2\overset{Cl}{C}HCH_2O\overset{O}{\underset{OCH_2\underset{Cl}{C}HCH_2Cl}{P}}OCH_2\overset{Cl}{C}HCH_2Cl$	++	✓				
A	2-Chlorobutane CAS No.: 78-86-4  $CH_3\underset{Cl}{C}HCH_2CH_3$	+	✓				
A	1,2-Dichloropropane CAS No.: 78-87-5  $ClCH_2\underset{Cl}{C}HCH_3$	+	✓		✓	✓ (E)	
A (5)	2,3-Dichloropropene CAS No.: 78-88-6  $CH_3\overset{Cl}{C}=CHCl$	++	✓			✓ (E)	
C	1,1,2-Trichloroethane CAS No.: 79-00-5 Cl_2CHCH_2Cl	C (NCI Bioassay)	✓		✓	✓ (E)	

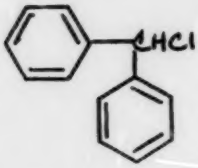
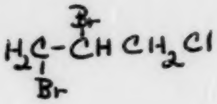
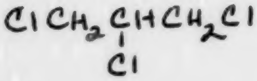
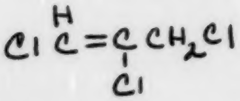
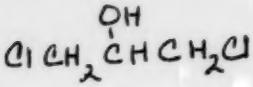
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
C (6)	Dichloroacetaldehyde CAS No.: 79-02-7  $Cl_2CHCH(=O)$	+	✓				
A (6)	Chloroacetyl chloride CAS No.: 79-04-9  $ClCH_2C(=O)Cl$	+	✓				
C	1,1,2,2-Tetrachloroethane CAS No.: 79-34-5 $Cl_2CHCHCl_2$	C (NCI Bioassay)	✓				
G	alpha,alpha,2,6-Tetra-chlorotoluene CAS No.: 81-19-6 	++	✓				
I	1-(Chloromethyl)naphthalene CAS No.: 86-52-2 	++	✓				

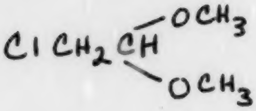
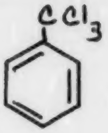
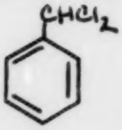
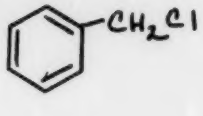
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Durr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
F	Chlorodiphenylmethane CAS No.: 90-99-3 	++	✓				
A	1,2-Dibromo-3-chloropropane CAS No.: 96-12-8  $H_2\underset{Br}{C}-\overset{Br}{C}HCH_2Cl$	C	✓			✓ (C)	
A	1,2,3-Trichloropropane CAS No.: 96-18-4  $ClCH_2\underset{Cl}{C}HCH_2Cl$	+	✓		✓	✓ (E)	
A (5)	1,2,3-Trichloropropene CAS No.: 96-19-5  $Cl\overset{H}{C}=\underset{Cl}{C}CH_2Cl$	++	✓			✓ (E/C)	
A	1,3-Dichloro-2-propanol CAS No.: 96-23-1  $ClCH_2\overset{OH}{C}HCH_2Cl$	+	✓				

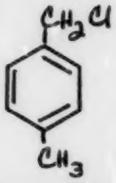
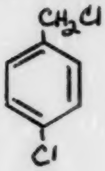
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) $EPA-H_2O$	(5) NCI(E/C)	(6) Other
A	3-Chloro-1,2-propanediol CAS No.: 96-24-2 $ClCH_2CH(OH)CH_2OH$	+	✓				
A	Chloroacetaldehyde, dimethyl acetal CAS No.: 97-97-2  $ClCH_2CH\begin{matrix}OCH_3\\OCH_3\end{matrix}$	++	✓				
G	*alpha*,*alpha*,*alpha*-Trichlorotoluene CAS No.: 98-07-7 	++	✓				
G	*alpha*,*alpha*-Dichlorotoluene CAS No.: 98-87-3 	++	✓				
F	*alpha*-Chlorotoluene (benzyl chloride) CAS No.: 100-44-7 	C?	✓	✓		✓ (C)	*IARC*, *11*, 217 *ACS*, p. 160

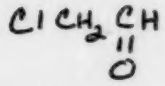
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcinogenicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
F	alpha-Chloro-p-xylene CAS No.: 104-82-5 	++	✓				
F	p,alpha-Dichlorotoluene CAS No.: 104-83-6 	++	✓				
A	3-Chloropropene CAS No.: 107-05-1 $ClCH_2CH=CH_2$	++	✓			✓ (E)	
A	1,2-Dichloroethane CAS No.: 107-06-2 $ClCH_2CH_2Cl$	+	✓	✓	✓	✓ (E)	ACS, p. 158
A	2-Chloroethanol CAS No.: 107-07-3 $ClCH_2CH_2OH$	+	✓	✓			ACS, p. 158

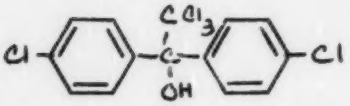
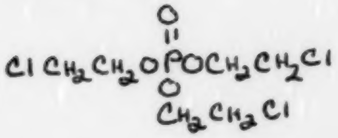
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
A (6)	Chloroacetaldehyde CAS No.: 107-20-0  $ClCH_2CH{=}O$	+	✓				
A	Chloromethyl methyl ether CAS No.: 107-30-2 $ClCH_2OCH_3$	C?	✓	✓		✓ (C)	IARC, 4, 239; ACS, p. 202
B	1-Chloro-3-methylbutane CAS No.: 107-84-6 $ClCH_2CH_2CH(CH_3)_2$	+	✓				
A	1-Chlorobutane CAS No.: 109-69-3 $ClCH_2CH_2CH_2CH_3$	+	✓			✓ (E)	
A	1-Bromo-3-chloropropane CAS No.: 109-70-6 $BrCH_2CH_2CH_2Cl$	+	✓				

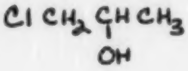
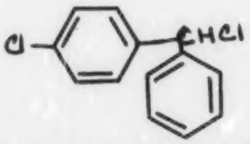
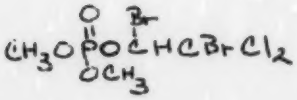
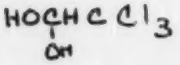
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino- genicity	(2) DCP- Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
A	2-Chloroethyl vinyl ether CAS No.: 110-75-8 $ClCH_2CH_2OCH=CH_2$	++	✓				
A (2)	bis(2-Chloroethyl)ether CAS No.: 111-44-4 $ClCH_2CH_2OCH_2CH_2Cl$	C?	✓	✓		✓ (C)	IARC, 9, 117
C	2,2,2-Trichloroethanol CAS No.: 115-20-8 Cl_3CCH_2OH	+	✓				
D	3,3'-Dichloro-a-(trichloromethyl) benzhydrol CAS No.: 115-32-2 	++	✓			✓ (E)	
A	2-Chloroethanol, phosphate CAS No.: 115-96-8  $ClCH_2CH_2O\overset{O}{\overset{\|}{\underset{\underset{CH_2CH_2Cl}{O}}{P}}}OCH_2CH_2Cl$	+	✓				

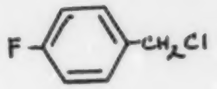
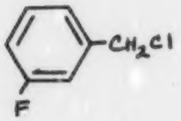
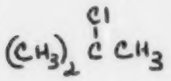
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
A	1-Chloro-2-propanol CAS No.: 127-00-4  $ClCH_2\underset{OH}{C}HCH_3$	+	✓	✓			
F	Chloro(p-chlorophenyl)phenylmethane CAS No.: 134-83-8 	++	✓				
C	2-Bromo-2-chloro-1,1,1-trifluoroethane (halothane) CAS No.: 151-67-7 $F_3CCHBrCl$	+	✓				
C	Phosphoric acid, 1,2-dibromo-2,2-dichloroethyl dimethyl ester CAS No.: 300-76-5  $CH_3O\overset{O}{\underset{OCH_3}{P}}O\overset{Br}{C}HCBrCl_2$	++	✓				
C	2,2,2-Trichloro-1,1-ethanediol (chloral hydrate) CAS No.: 302-17-0  $HO\underset{OH}{C}HCCl_3$	++	✓			✓ (E)	

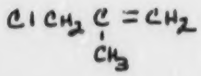
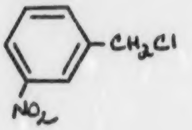
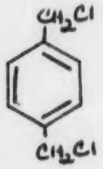
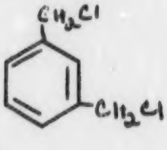
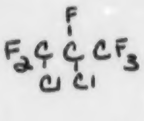
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
F	p-Fluorobenzyl chloride CAS No.: 352-11-4 	+	✓				
F	m-Fluorobenzyl chloride CAS No.: 456-42-8 	+	✓				
A	2-Chloro-2-methylpropane CAS No.: 507-20-0  $(CH_3)_2\overset{Cl}{C}CH_3$	C?	✓			✓ (E)	Poirier, L., et al., Cancer Res. 35, 1411, 1975
A	n-Propyl chloride CAS No.: 540-54-5 $CH_3CH_2CH_2Cl$	+	✓				
A (5)	1,3-Dichloropropene CAS No.: 542-75-6 $ClCH=CHCH_2Cl$	++	✓		✓		

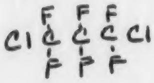
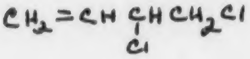
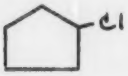
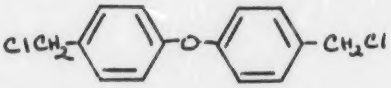
ALKYL HALIDES (continued)

I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
A	3-Chloro-2-methyl-1-propene CAS No.: 563-47-3  $ClCH_2\underset{CH_3}{C}=CH_2$	++	✓			✓ (E)	
F (7)	*alpha*-Chloro-*m*-nitrotoluene CAS No.: 619-23-8 	++	✓				
F (2)	*para*-Dichloroxylene CAS No.: 623-25-6 	++	✓				
F (2)	*meta*-Dichloroxylene CAS No.: 626-16-4 	++	✓				
C	1,2-Dichlorohexafluoropropane CAS No.: 661-97-2  $F_2\underset{Cl}{C}\overset{F}{\underset{Cl}{C}}CF_3$	0	✓				

ALKYL HALIDES (continued)

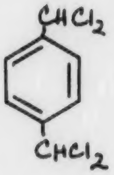
I. CHLORIDES (continued)

Structure Class		(1) Carcino- genicity	(2) DCP- Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
C	1,3-Dichlorohexafluoropropane CAS No.: 662-01-1  $\mathrm{Cl\overset{F}{\underset{F}{C}}\overset{F}{\underset{F}{C}}\overset{F}{\underset{F}{C}}Cl}$	0	✓				
A	3,4-Dichlorobutene-1 CAS No.: 760-23-6  $\mathrm{CH_2{=}CH\,\underset{Cl}{CH}CH_2Cl}$	++	✓				
E	Cyclopentyl chloride CAS No.: 930-28-9 	++	✓				
F (2)	para-Chloromethyl diphenyl oxide CAS No.: 2362-18-7 	++	✓				
C	1,1-Dichloromethyl methyl ether CAS No.: 4885-02-3 $\mathrm{Cl_2CHOCH_3}$	C?	✓			✓ (C)	ACS, p. 204

ALKYL HALIDES (continued)

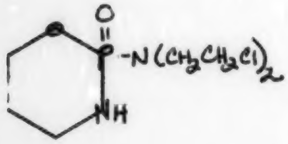
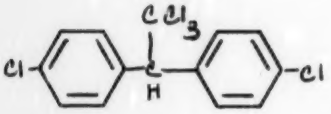
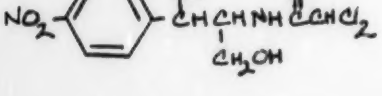
I. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
G (2)	*alpha*,*alpha*,*alpha*,*alpha*-Tetrachloroparaxylene CAS No.: 7398-82-5	++	✓				



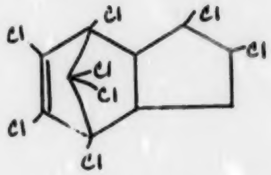
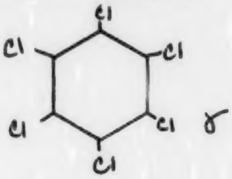
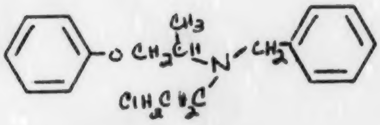
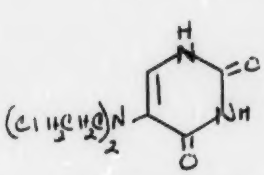
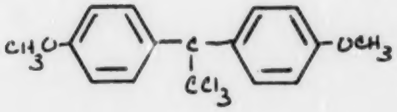
ALKYL HALIDES (continued)

I.A. CHLORIDES

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
B	Cyclophosphamide CAS No.: 50-18-0 	C				✓ (C)	IARC, 9, 135; ACS, p. 214
D	1,1,1-Trichloro-2,2-bis(p-chlorophenyl)ethane (DDT) CAS No.: 50-29-3 	C?			✓	✓ (E/C)	IARC, 5, 83; ACS, p. 162
H (2)	Nitrogen mustard CAS No.: 51-75-2 $CH_3N(CH_2CH_2Cl)_2$	C				✓ (C)	IARC, 9, 193
H (2)	Nitrogen mustard·HCl CAS No.: 55-86-7 $CH_3N(CH_2CH_2Cl)_2 \cdot HCl$	C				✓ (C)	IARC, 9, 193; ACS, p. 208
D	Chloramphenicol CAS No.: 56-75-7 	C? (leukemogenic activity--probably not a result of labile halide)				✓ (C)	IARC, 10, 85

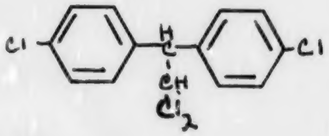
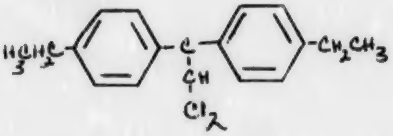
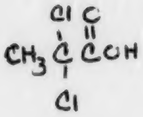
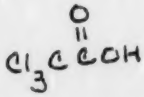
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
E (5)	Chlordane CAS No.: 57-74-9 	C (NCI Bioassay)			✓	✓ (E)	
E	1,2,3,4,5,6-Hexachloro (gamma)-cyclohexane (Lindane) CAS No.: 58-89-9 	C?			✓	✓ (E)	IARC, 5, 47
H	Phenoxybenzamine CAS No.: 59-96-1 	C?					IARC, 9, 223
H (1)	Uracil mustard CAS No.: 66-75-1 	C				✓ (C)	IARC, 9, 235; ACS, p. 214
D	Methoxychlor CAS No.: 72-43-5 	++				✓ (E)	IARC, 5, 193

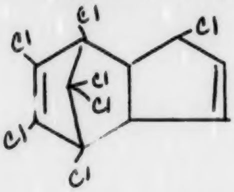
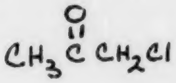
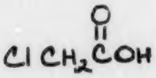
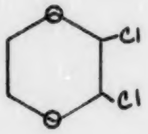
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
D	1,1-Dichloro-2,2-bis(*p*-chlorophenyl)ethane CAS No.: 72-54-8 	C?				✓ (E)	*IARC*, *5*, 83
D	Perthane CAS No.: 72-56-0 	++				✓ (E)	
C (6)	Dalapon CAS No.: 75-99-0  $CH_3\overset{Cl}{\underset{Cl}{C}}\overset{O}{\overset{\|}{C}}OH$	+				✓ (E)	
C (6)	Trichloroacetic acid CAS No.: 76-03-9  $Cl_3C\overset{O}{\overset{\|}{C}}OH$	+				✓ (E)	
C	Difluorotetrachloroethane CAS No.: 76-11-9 ClF_2CCCl_3	+				✓ (E)	

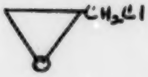
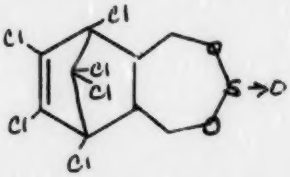
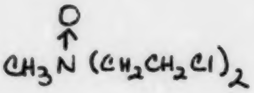
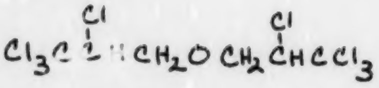
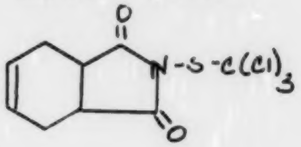
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino- genicity	(2) DCP- Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
C	Freon 113 CAS No.: 76-13-1 $Cl_2FCCClF_2$	0				✓ (C)	ACS, p. 158
E (5)	Heptachlor CAS No.: 76-44-8 	C (NCI Bioassay)			✓	✓ (E)	IARC, 5, 173
A	Chloroacetone CAS No.: 78-95-5  $CH_3C(=O)CH_2Cl$	C?				✓ (C)	ACS, p. 160
A	Chloroacetic acid CAS No.: 79-11-8  $ClCH_2C(=O)OH$	+				✓ (C)	ACS, p. 160
E	2,3-Dichloro-1,4-dioxane CAS No.: 95-59-0 	C?				✓ (C)	

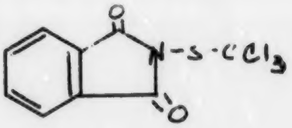
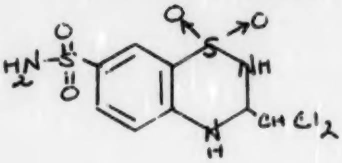
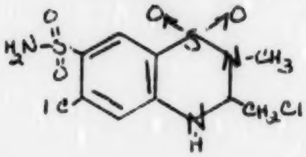
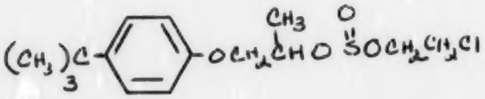
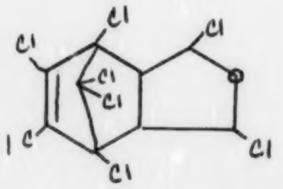
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
A (3)	Epichlorohydrin CAS No.: 106-89-8 	C?		✓		✓ (E/C)	IARC, 11, 131; ACS, p. 174
E (5)	Endosulfan (Thiodan) CAS No.: 115-29-7 	++				✓ (E/C)	
H (2)	Nitrogen Mustard -oxide CAS No.: 126-85-2  $CH_3\overset{\overset{O}{\uparrow}}{N}(CH_2CH_2Cl)_2$	C?				✓ (C)	IARC, 9, 209; ACS, p. 210
D (2)	bis(2,3,3,3-Tetrachloropropyl) ether CAS No.: 127-90-2  $Cl_3C\overset{Cl}{C}HCH_2OCH_2\overset{Cl}{C}HCCl_3$	C?				✓ (C)	ACS, p. 204
D	Captan CAS No.: 133-06-2 	+				✓ (C)	

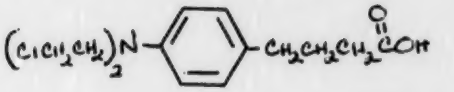
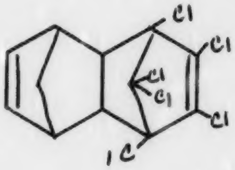
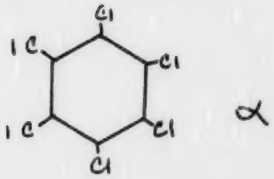
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
D	Folpet CAS No.: 133-07-3 	+				✓ (C)	
D	Trichlormethiazide CAS No.: 133-67-5 	+				✓ (E)	
B	Methyclothiazide CAS No.: 135-07-9 	+				✓ (E)	
	β-ρ-t-Butyl phenoxy-α-methyl-β-chlorodiethyl sulfite CAS No.: 140-57-8 	C				✓ (C)	IARC, 5, 39
E (3)	Telodrin CAS No.: 297-78-9 	++				✓ (C)	

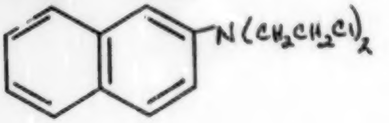
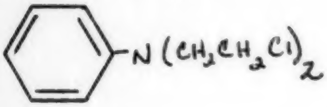
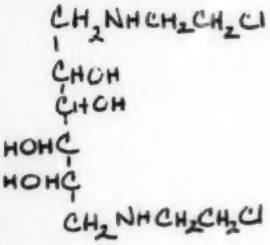
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
H (2)	N,N-Di-(2-Chloroethyl)-p-aminophenyl butyric acid (Chloroambucil) CAS No.: 305-03-3 	C?				✓ (C)	IARC, 9, 125; ACS, p. 210
E (5)	Aldrin CAS No.: 309-00-2 	C (NCI Bioassay)			✓	✓ (E/C)	IARC, 5, 25; ACS, p. 210
E	1,2,3,4,5,6-Hexachloro(alpha)-cyclohexane CAS No.: 319-84-0 	C?					IARC, 5, 47
C	Trichlorotrifluoroethane CAS No.: 354-58-5 Cl_3CCF_3	0			✓	✓ (E)	
A (2)	bis(Chloromethyl)ether CAS No.: 432-88-1 $ClCH_2OCH_2Cl$	C		✓		✓ (C)	IARC, 4, 231; ACS, p. 202

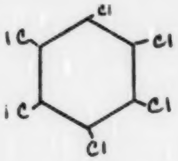
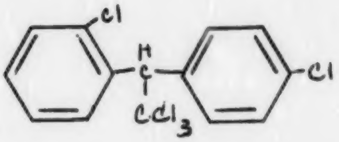
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Dari	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
H (2)	N,N-bis(2-Chloroethyl)-2-naphthylamine CAS No.: 494-03-1 	C				✓ (C)	IARC, 4, 119; ACS, p. 212
H (2)	β,β'-Dichlorodiethyl sulfide CAS No.: 505-60-2 $S(CH_2CH_2Cl)_2$	C?				✓ (C)	IARC, 9, 181; ACS, p. 208
H (2)	N,N-Di(2-Chloroethyl)aniline CAS No.: 553-27-5 	C?					ACS, p. 212
H	1,6-bis((2-Chloroethyl)amino)-1,6-dideoxy-d-mannitol dihydrochloride CAS No.: 576-68-1  $CH_2NHCH_2CH_2Cl$ $CHOH$ $CHOH$ $HOHC$ $HOHC$ $CH_2NHCH_2CH_2Cl$	C?				✓ (C)	IARC, 9, 157; ACS p. 212 (not the HCl)

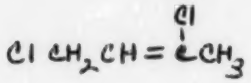
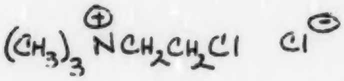
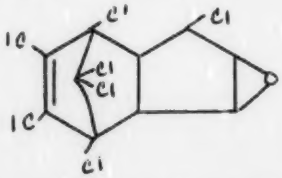
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino- genicity	(2) DCP- Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
E	Hexachlorocyclohexane (technical BHC) CAS No.: 608-73-1 	C?				✓ (C)	IARC, 5, 47
B	Chloroacetaldehyde, diethyl acetal CAS No.: 621-62-5 $ClCH_2CH(OCH_2CH_3)_2$	N				✓ (C)	ACS, p. 204
C	Chlorodifluoromethane CAS No.: 754-45-6 F_2CHCl	0				✓ (E)	
A (2)	1,4-Dichloro-2-butene CAS No.: 764-41-0 $ClCH_2CH=CHCH_2Cl$	++				✓ (E)	
D	o,p'-Dichlorodiphenyltrichloroethane CAS No.: 789-02-6 	++					IARC, 5, 83

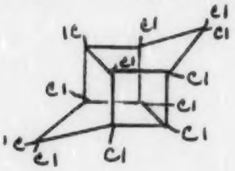
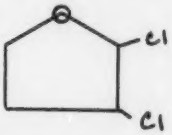
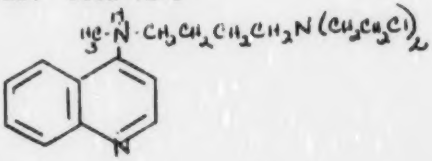
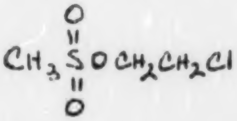
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
H (2)	Trichlorotriethylamine hydrochloride CAS No.: 817-09-4 $N(CH_2CH_2Cl)_3 \cdot HCl$	C?					IARC, 9, 229; ACS, p. 210
A (5)	1,3-Dichloro-2-butene CAS No.: 926-57-8  $ClCH_2CH=\overset{Cl}{C}CH_3$	++				✓ (E)	
H	(2-Chloroethyl)-trimethylammonium chloride CAS No.: 999-81-5  $(CH_3)_3\overset{\oplus}{N}CH_2CH_2Cl \quad Cl^{\ominus}$	++					ACS, p. 204
E (3,5)	Heptachlor epoxide CAS No.: 1024-57-3 	C			✓	✓ (E)	Fed. Reg. 49 11/26 1974
C	Dichlorotetrafluoroethane CAS No.: 1320-37-2 Cl_2FCCF_3	0				✓ (E)	

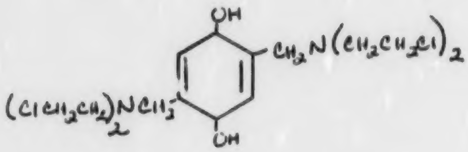
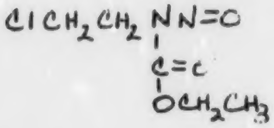
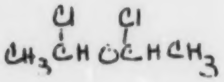
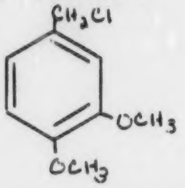
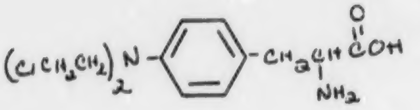
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
C	Chlorotrifluoromethane CAS No.: 1330-45-6 $ClCF_3$	0				✓ (E)	
E	Mirex CAS No.: 2385-85-5  Cl Cl Cl Cl Cl Cl Cl Cl Cl Cl Cl Cl	C?				✓ (C)	IARC, 5, 203
E	2,3-Dichlorotetrahydrofuran CAS No.: 3511-19-1 	C?				✓ (C)	
H (2)	4-(4-(Di-(2-Chloroethyl)amino)-1-methylbutylamino)-7-chloroquinoline (Chloroquine mustard) CAS No: 3562-71-8  $H_3C \cdot \overset{H}{N} \cdot CH_2CH_2CH_2CH_2N(CH_2CH_2Cl)_2$ N	C?					ACS, p. 214
A	Methane sulfonic acid, 2-chloroethyl ester CAS No.: 3570-58-9  $CH_3\overset{O}{\underset{O}{S}}OCH_2CH_2Cl$	++				✓ (C)	ACS, p. 206

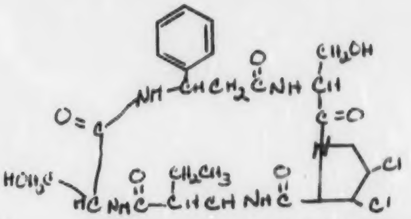
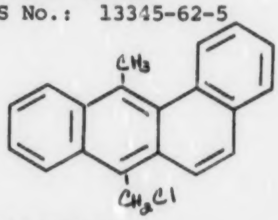
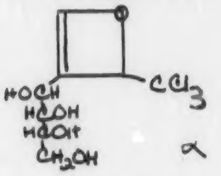
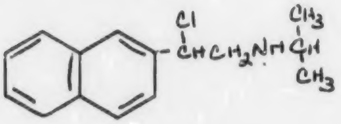
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
H (2)	2,5-bis(bis(2-Chloroethyl)amino)-methyl hydroquinone CAS No.: 4420-79-5 	C?				✓ (C)	ACS, p. 212
H (7)	N-(2-Chloroethyl)-N-nitroso-urethane CAS No.: 6296-45-3  $ClCH_2CH_2\underset{\underset{\underset{OCH_2CH_3}{\vert}}{C=C}}{\vert}{N}N{=}O$	C?					ACS, p. 204
A (2)	bis(1-Chloroethyl)ether CAS No.: 6986-48-7  $CH_3\overset{Cl}{C}H\,O\overset{Cl}{C}HCH_3$	C?				✓ (C)	
F	α-Chloro-3,4-dimethoxy toluene CAS No.: 7306-46-9 	N				✓ (C)	ACS, p. 160
H (2)	p-Di-(2-Chloroethyl)amino-d-phenylalanine CAS No.: 10345-94-8 	C				✓ (C)	IARC, 9, 167

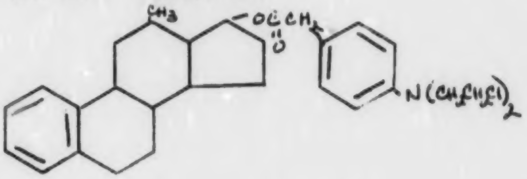
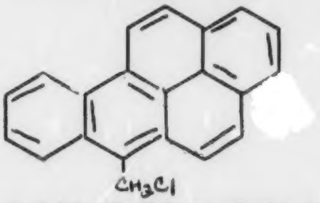
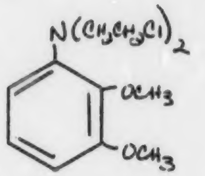
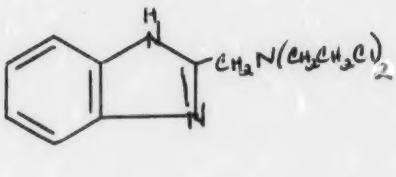
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
E	Cyclochlorotine CAS No.: 12663-46-6 	C?				✓ (C)	IARC, 10, 139
I (4)	7-Chloromethyl-12-methylbenz-(a)anthracene CAS No.: 13345-62-5 	C?				✓ (C)	ACS, p. 164
D	α-Chloralose CAS No.: 15879-93-3 	+				✓ (C)	
I	β-Chloro-N-isopropyl-2-naphthalene ethylamine·HCl CAS No.: 20794-96-1 	C?				✓ (C)	

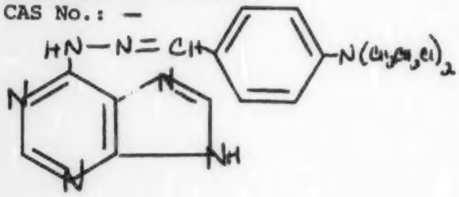
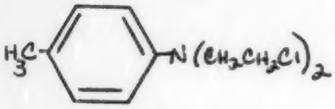
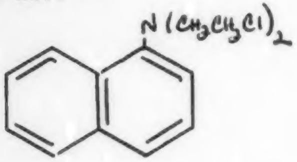
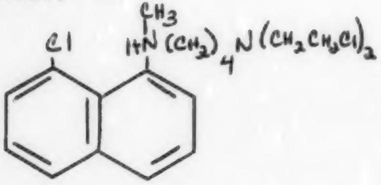
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
H (2)	(0)estradiol mustard CAS No.: 22966-79-6 	C?					IARC, 9, 217
I (4)	6-Chloromethylbenzo(a)pyrene CAS No.: 49852-84-8 	C?				✓ (C)	ACS, p. 258
H (2)	N,N-bis(2-Chloroethyl)-2,3-dimethoxyaniline CAS No.: — 	C?				✓ (C)	ACS, p. 107
H (1,2)	Benzimidazole mustard CAS No.: — 	C?				✓ (C)	ACS, p. 214

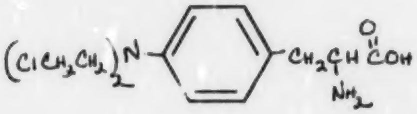
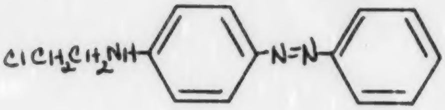
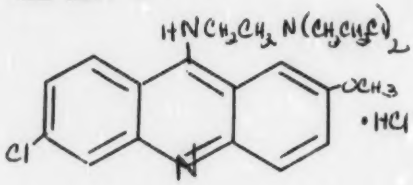
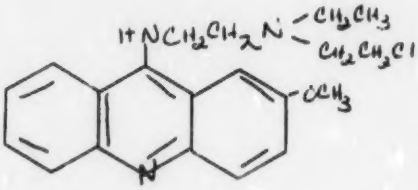
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
H (1,2)	Benzalpurine mustard CAS No.: —  HN—N=CH N(CH₂CH₂Cl)₂ N N N NH	++					ACS, p. 216
H (2)	N,N-Di-(2-Chloroethyl)-p-toluidine CAS No.: —  H₃C N(CH₂CH₂Cl)₂	C?					ACS, p. 212
H (2)	N,N-Di(2-Chloroethyl)-1-naphthyl-amine CAS No.: —  N(CH₂CH₂Cl)₂	C?					ACS, p. 212
H (2)	4-(4-(Di-(2-Chloroethyl)amino)-1-methylbutylamino)-5-chloro-quinoline (5-Quinoline mustard) CAS No.: —  CH₃ Cl HN(CH₂)₄N(CH₂CH₂Cl)₂	++					ACS, p. 216

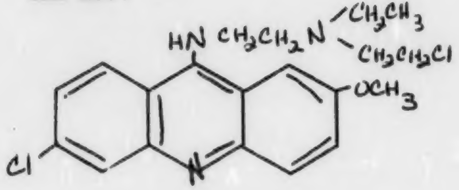
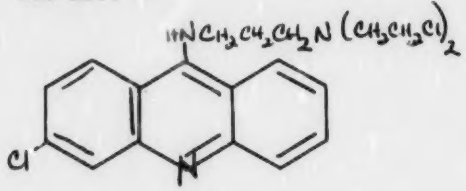
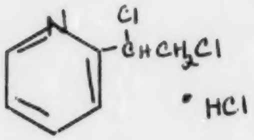
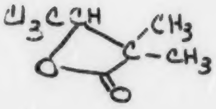
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
H (2)	p-Di-(2-Chloroethyl)amino-1-phenylalanine CAS No.: — 	C?					ACS, p. 107
H (7)	N-(2-Chloroethyl)aminoazobenzene CAS No.: — 	++					ACS, p. 204
H (2,4)	Quinacrine ethyl mustard CAS No.: — 	C?				✓ (C)	ACS, p. 214
H (4)	Quinacrine ethyl half mustard CAS No.: — 	C?				✓ (C)	ACS, p. 204

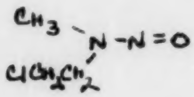
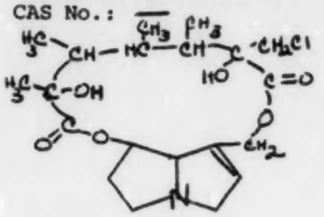
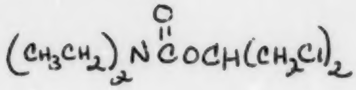
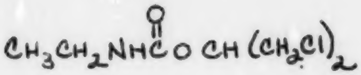
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
H (4)	9-(3-(Ethyl-2-chloroethyl)amino-ethylamino)-6-chloro-2-methoxy-acridine CAS No.: —  HN CH₂CH₂N CH₂CH₃ CH₂CH₂Cl OCH₃ Cl N	++					ACS, p. 204
H (2,4)	Quinacrinepropyl mustard CAS No.: —  HNCH₂CH₂CH₂N (CH₂CH₂Cl)₂ Cl N	++					ACS, p. 214
F, B	2-(α,β-Dichloroethyl)pyridine hydrochloride CAS No.: —  N Cl CHCH₂Cl · HCl	C?				✓ (C)	
D	3-Hydroxy-2,2-dimethyl-4,4,4-trichlorobutyric acid β-lactone CAS No.: —  Cl₃C CH CH₃ C–CH₃ O O	+					ACS, p. 196

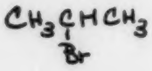
ALKYL HALIDES (continued)

I.A. CHLORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
H (7)	N-Nitrosomethyl-2-chloroethylamine CAS No.: – 	C?					ACS, p. 522
B	Chlorodeoxysceleratine CAS No.: — 	+					ACS, p. 630
A (7)	2,2'-Dichloroisopropyl-N,N-diethyl carbamate CAS No.: ——  $(CH_3CH_2)_2N\overset{\overset{O}{\|}}{C}OCH(CH_2Cl)_2$	C?				✓ (C)	
A (7)	2,2'-Dichloro isopropyl-N -ethyl-carbamate CAS No.: ——  $CH_3CH_2NH\overset{\overset{O}{\|}}{C}OCH(CH_2Cl)_2$	C?				✓ (C)	

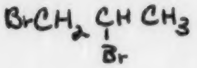
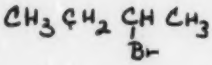
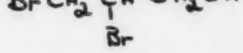
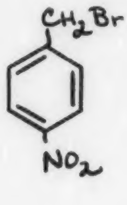
ALKYL HALIDES (continued)

II. BROMIDES

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
C	Dibromomethane CAS No.: 74-95-3 CH_2Br_2	++	✓				
A	Bromoethane CAS No.: 74-96-4 CH_3CH_2Br	+	✓			✓ (C)	
C	Tribromomethane CAS No.: 75-25-2 $CHBr_3$	++	✓				
A	2-Bromopropane CAS No.: 75-26-3  $CH_3\underset{Br}{C}HCH_3$	+	✓				
C	Dibromodifluoromethane CAS No.: 75-61-6 F_2CBr_2	+	✓				

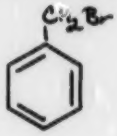
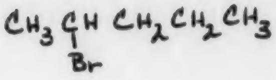
ALKYL HALIDES (continued)

II. BROMIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
C	Bromotrifluoromethane CAS No.: 75-63-8 $BrCF_3$	0	✓				
A	1,2-Dibromopropane CAS No.: 78-75-1  $BrCH_2\underset{Br}{CH}CH_3$	++	✓				
A	2-Bromobutane CAS No.: 78-76-2  $CH_3CH_2\underset{Br}{CH}CH_3$	C?	✓			✓ (C)	Poirier,L. et al., Cancer Res. 35,1114, 1975
C	1,1,2,2-Tetrabromoethane CAS No.: 79-27-6 $Br_2CHCHBr_2$	++	✓				
A	2,3-Dibromo-1-propanol CAS No.: 96-13-9  $BrCH_2\underset{Br}{CH}CH_2OH$	+	✓		✓		
F (7)	alpha-Bromo-p-nitrotoluene CAS No.: 100-11-8 	+	✓				

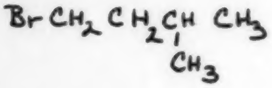
ALKYL HALIDES (continued)

II. BROMIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
F	alpha-Bromotoluene CAS No.: 100-39-0 	++	✓				
A	1,2-Dibromoethane CAS No.: 106-93-4 $BrCH_2CH_2Br$	C	✓	✓		✓ (C)	ACS, p. 158
A	1-Bromopropane CAS No.: 106-94-5 $BrCH_2CH_2CH_3$	++	✓				
A	3-Bromopropene CAS No.: 106-95-6 $BrCH_2CH=CH_2$	++	✓				
B	2-Bromopentane CAS No.: 107-81-3  $CH_3\underset{\mathrm{Br}}{\underset{\vert}{C}}H\,CH_2CH_2CH_3$	+	✓				

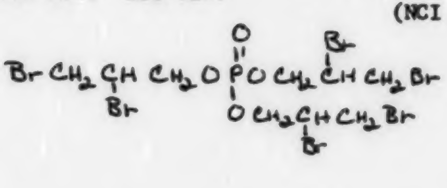
ALKYL HALIDES (continued)

II. BROMIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
B	1-Bromo-3-methylbutane CAS No.: 107-82-4  $BrCH_2CH_2\underset{CH_3}{CH}CH_3$	+	✓				
A (2)	1,3-Dibromopropane CAS No.: 109-64-8 $BrCH_2CH_2CH_2Br$	+	✓				
A	1-Bromobutane CAS No.: 109-65-9 $BrCH_2CH_2CH_2CH_3$	+	✓		✓	✓ (C)	
A (2)	1,4-Dibromobutane CAS No.: 110-52-1 $BrCH_2CH_2CH_2CH_2Br$	+	✓				

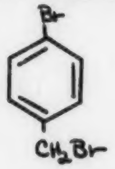
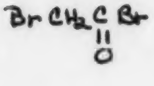
ALKYL HALIDES (continued)

II. BROMIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
B	1-Bromopentane CAS No.: 110-53-2 $Br(CH_2)_4CH_3$	+	✓				
B (2)	1,5-Dibromopentane CAS No.: 111-24-0 $Br(CH_2)_5Br$	+	✓				
C	1,2-Dibromotetrafluoroethane CAS No.: 124-73-2 BrF_2CCF_2Br	0	✓				
A	2,3-Dibromo-1-propanol, phosphate CAS No.: 126-72-7  $Br{-}CH_2\underset{Br}{CH}CH_2O\overset{O}{\underset{OCH_2\underset{Br}{CH}CH_2Br}{P}}OCH_2\overset{Br}{CH}CH_2Br$	C (NCI Bioassay)	✓				

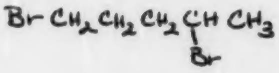
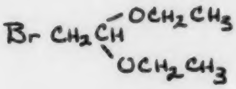
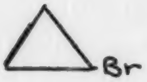
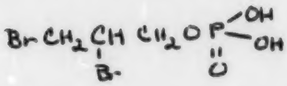
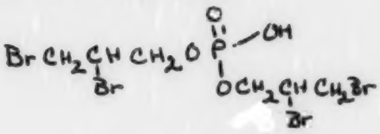
ALKYL HALIDES (continued)

II. BROMIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
A	2-Bromoethanol CAS No.: 540-51-2 $Br-CH_2CH_2OH$	+	✓				
C	Tetrabromomethane CAS No.: 558-13-4 CBr_4	++	✓				
F	Benzene, 1-bromo-4-(bromomethyl)- CAS No.: 589-15-1 	++	✓				
A (6)	Bromoacetyl bromide CAS No.: 598-21-0  $BrCH_2\overset{\displaystyle O}{\overset{\parallel}{C}}Br$	+	✓				

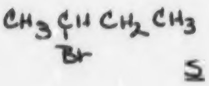
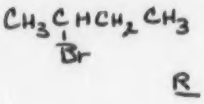
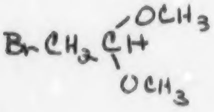
ALKYL HALIDES (continued)

II. BROMIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
B (2)	1,4-Dibromopentane CAS No.: 626-87-9  $\mathrm{Br{-}CH_2CH_2CH_2\underset{Br}{CH}\,CH_3}$	+	✓				
B	Bromoacetaldehyde, diethyl acetal CAS No.: 2032-35-1 	++	✓				
E	Cyclopropyl bromide CAS No.: 4333-56-6 	+	✓				
A	mono-(2,3-Dibromopropyl) Phosphoric acid CAS No.: 5324-12-9 	++	✓				
A	bis(2,3-Dibromopropyl) Phosphoric acid CAS No.: 5412-25-9 	++	✓				

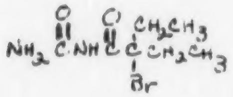
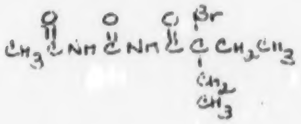
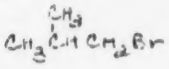
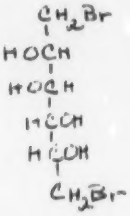
ALKYL HALIDES (continued)

II. BROMIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
A	2-Bromobutane, (S)- CAS No.: 5787-32-6  $CH_3\underset{Br}{C}HCH_2CH_3$ $\underline{S}$	C?	✓			✓ (C)	Poirier, L. et al., Cancer Res. 35, 1114, 1975
A	2-Bromobutane, (R)- CAS No.: 5787-33-7  $CH_3\underset{Br}{C}HCH_2CH_3$ $\underline{R}$	"	✓			✓ (C)	
A	Dimethylbromoacetal CAS No.: 7252-83-7  $BrCH_2\overset{OCH_3}{\underset{OCH_3}{C}}H$	++	✓				

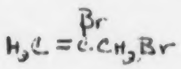
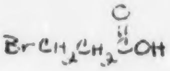
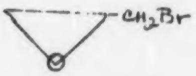
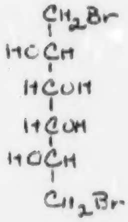
ALKYL HALIDES (continued)

II.A. BROMIDES

Structure Class		(1) Carcino- genicity	(2) DCP- Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
A	Methyl bromide CAS No.: 74-83-9 CH_3Br	+			✓	✓ (C)	ACS, p. 156
B	Carbromal CAS No.: 77-65-6  $NH_2\overset{O}{\overset{\|}{C}}NH\overset{O}{\overset{\|}{C}}\underset{Br}{\overset{CH_2CH_3}{C}}CH_2CH_3$	++				✓ (E/C)	
B	Acetylcarbromal CAS No.: 77-66-7  $CH_3\overset{O}{\overset{\|}{C}}NH\overset{O}{\overset{\|}{C}}NH\overset{O}{\overset{\|}{C}}\underset{\underset{CH_3}{CH_2}}{\overset{Br}{C}}CH_2CH_3$	++				✓ (E)	
A	1-Bromo-2-methylpropane CAS No.: 78-77-3  $CH_3\overset{CH_3}{CH}CH_2Br$	C?				✓ (C)	Poirier, L., et al., Cancer Res. 35, 1114, 1975
B (2)	Dibromomannitol CAS No.: 488-41-5 	C?				✓ (C)	

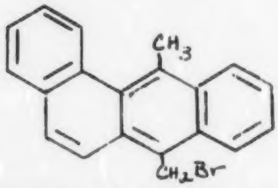
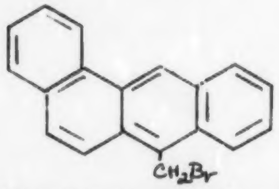
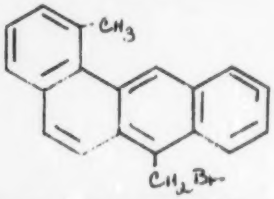
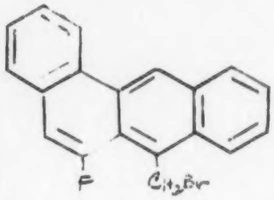
ALKYL HALIDES (continued)

II.A. BROMIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
A	2-Bromo-2-methylpropane CAS No.: 507-19-7 $(CH_3)_3CBr$	C				✓ (C)	Poirier, L. et al., Cancer Res. 35, 1114, 1975
A (5)	2,3-Dibromopropylene CAS No.: 513-31-5  $H_2C{=}\overset{Br}{C}\cdot CH_2Br$	++			✓		
A (6)	3-Bromopropionic acid CAS No.: 590-92-1  $BrCH_2CH_2\overset{O}{\overset{\Vert}{C}}OH$	C?				✓ (C)	ACS, p. 160
A (3)	Epibromohydrin CAS No.: 3132-64-7 	++				✓ (C)	ACS, p. 177
B (2)	Dibromodulcitol CAS No.: 10318-26-0 	C?				✓ (C)	

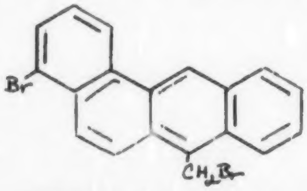
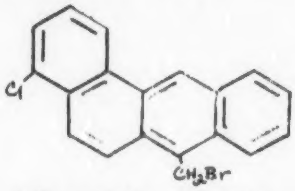
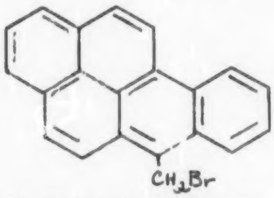
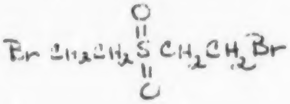
ALKYL HALIDES (continued)

II.A. BROMIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
I (4)	7-Bromomethyl-12-methylbenz-(a)anthracene CAS No.: 16238-56-5  	C				✓ (C)	ACS, p. 162
I (4)	7-Bromomethylbenz(a)anthracene CAS No.: 24961-39-5  	C				✓ (C)	ACS, p. 162
I (4)	1-Methyl-7-bromomethylbenz-(a)anthracene CAS No.: 34346-96-8  	C?				✓ (C)	ACS, p. 162
I (4)	6-Fluoro-7-bromomethylbenz-(a)anthracene CAS No.: 34346-97-9  	C?				✓ (C)	

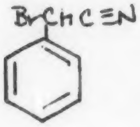
ALKYL HALIDES (continued)

II.A. BROMIDES (continued)

Structure Class		(1) Carcino- genicity	(2) DCP- Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
I (4)	4-Bromo-7-bromomethylbenz-(a)anthracene CAS No.: 34346-98-0  	C?				✓ (C)	ACS, p. 162
I (4)	4-Chloro-7-bromomethylbenz-(a)anthracene CAS No.: 34346-99-1  	C?				✓ (C)	ACS, p. 162
I (4)	6-Bromomethylbenzo(α)pyrene CAS No.: 49852-85-9  	C?				✓(C)	
H (2)	β,β'-Bromodiethylsulfone CAS No.:  $BrCH_2CH_2\overset{O}{\underset{O}{\overset{\|\|}{\underset{\|\|}{S}}}}CH_2CH_2Br$	+				✓ (C)	

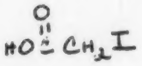
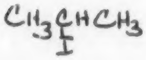
ALKYL HALIDES (continued)

II.A. BROMIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
H (2)	β,β'-Dibromodiethylsulfide CAS No.: $BrCH_2CH_2SCH_2CH_2Br$	++				✓ (C)	
F	α-Bromobenzyl cyanide CAS No.: — 	+				✓ (C)	

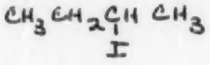
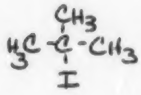
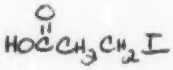
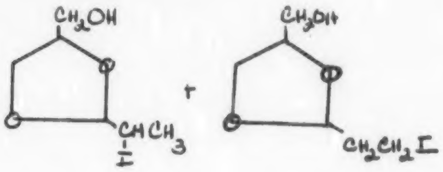
ALKYL HALIDES (continued)

III. IODIDES

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
A (6)	Iodoacetic acid CAS No.: 64-69-7  $HOC(=O)CH_2I$	+				✓ (C)	ACS, p. 160
A	Methyl iodide CAS No.: 74-88-4 CH_3I	C?			✓	✓(C)	ACS, p. 156
A	Ethyl iodide CAS No.: 75-03-6 CH_3CH_2I	+				✓ (C)	
A	Isopropyl iodide CAS No.: 75-30-9  CH_3CHICH_3	C?				✓ (C)	
A	n-Propyl iodide CAS No.: 107-08-4 $CH_3CH_2CH_2I$	C?				✓ (C)	

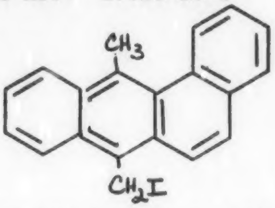
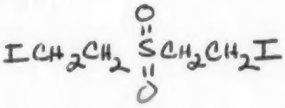
ALKYL HALIDES (continued)

III. IODIDES (continued)

Structure Class		(1) Carcino- genicity	(2) DCP- Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
A	2-Iodo-butane CAS No.: 513-48-4  $CH_3CH_2\underset{I}{CH}CH_3$	C?				✓ (C)	Poirier,L. et al., Cancer Res 35,1114, 1975
A	n-Butyliodide CAS No.: 542-69-8 $CH_3CH_2CH_2CH_2I$	C?				✓ (C)	Poirier,L. et al., Cancer Res. 35, 1114, 1975
A	t-Butyliodide CAS No.: 558-17-8  $H_3C-\overset{CH_3}{\underset{I}{C}}-CH_3$	++				✓ (C)	
A (6)	3-Iodopropionic acid CAS No.: 1417-64-3  $HO\overset{O}{\overset{\|}{C}}CH_3CH_2I$	C?				✓ (C)	ACS, p. 160
B	1,3-Dioxolane-4-methanol, (1- + 2-iodoethyl) CAS No.: 5634-39-9 	+				✓ (E)	

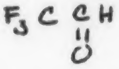
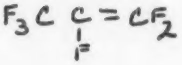
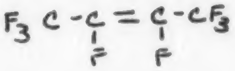
ALKYL HALIDES (continued)

III. IODIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
I (4)	7-(Iodomethyl)-12-methylbenz-(a)anthracene CAS No.: 27018-50-4 	C?				✓ (C)	ACS, p. 164
A (2)	β,β'-Diiododiethyl sulfone CAS No.: —  $ICH_2CH_2\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}CH_2CH_2I$	+				✓ (C)	

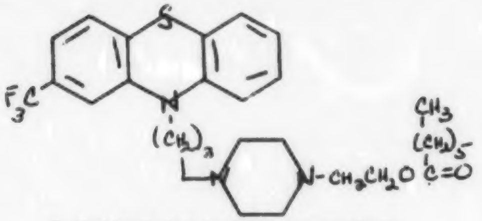
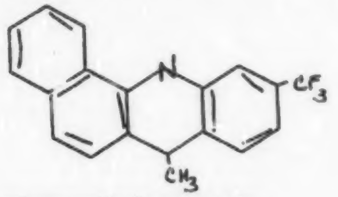
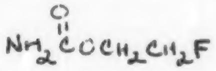
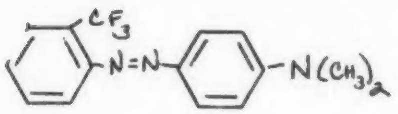
ALKYL HALIDES (continued)

IV. FLUORIDES

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
C (6)	Trifluoroacetaldehyde CAS No.: 75-90-1  $F_3C\underset{\overset{\|}{O}}{C}H$	0	✓				
C (5)	Hexafluoropropene CAS No.: 116-15-4  $F_3C\underset{\overset{\mid}{F}}{C}=CF_2$	+	✓				
C (5)	Perfluorobutene-2 CAS No.: 360-89-4  $F_3C-\underset{\overset{\mid}{F}}{C}=\underset{\overset{\mid}{F}}{C}-CF_3$	+	✓				

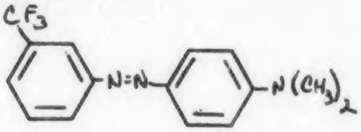
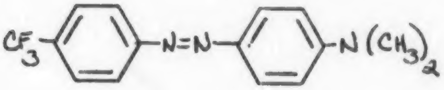
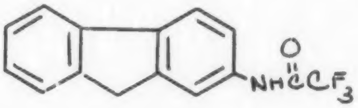
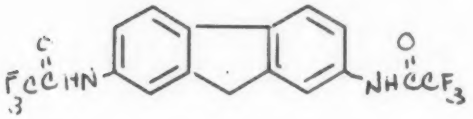
ALKYL HALIDES (continued)

IV.A. FLUORIDES

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
I (4)	Fluphenazine enanthate CAS No.: 2746-81-8 	0				✓ (E)	
I (4)	7-Methyl-10-trifluoromethyl-benz(c)acridine CAS No.: 5101-37-1 	0				✓ (C)	
A (7)	Fluoroethylcarbamate CAS No.: —  $NH_2\overset{\overset{O}{\|}}{C}OCH_2CH_2F$	+				✓ (C)	
G (7)	2'-Trifluoromethyl-4-dimethyl-aminoazobenzene CAS No.: - 	+				✓ (C)	

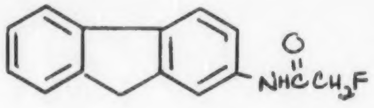
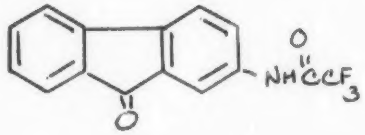
ALKYL HALIDES (continued)

IV.A. FLUORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
G (7)	3'-Trifluoromethyl-4-dimethyl-aminoazobenzene CAS No.: — 	+				✓ (C)	
G (7)	4'-Trifluoromethyl-4-dimethyl-aminoazobenzene CAS No.: — 	+				✓ (C)	
I (6)	2,2,2-Trifluoro-N-(fluorenyl)-2-acetamide CAS No.: — 	C?				✓ (C)	ACS, p. 400
I (6)	N,N'-fluorenyl-2,7-bis(tri-fluoroacetamide) CAS No.: — 	C?				✓ (C)	

ALKYL HALIDES (continued)

IV.A. FLUORIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI(E/C)	(6) Other
I (6)	N-(2-Fluorenyl)-2-fluoroacetamide CAS No.: — 	C?				✓ (C)	
I (6)	2,2,2-Trifluoro-n-(9-oxofluorenyl)-2-acetamide CAS No.: 	C?				✓ (C)	

C. Vinyl Halides

Because the majority of vinyl halides tested have been reported to be carcinogenic, all vinyl halides are regarded as suspect.

Vinyl halides containing only fluorine may be regarded with somewhat less suspicion because of the general lack of reactivity of C-F compounds.

Key to Interpretation of Vinyl Halides Table

Structure Class

A = Aliphatic
C = Cyclic

(1) Carcinogenicity

C = substantial human or animal experimental evidence
C? = limited evidence
N = negative in a reliable test
+ = for S/A reasons limited suspicion of carcinogenicity, e.g., F only
++ = for S/A reasons strong suspicion of carcinogenicity, e.g., all other halides
0 = no adequate experimental evidence and no compelling S/A analogy on which to base evaluation

(2) DCP-Darr - cited on list obtained by Darr from search of SRI-DCP data base

(3) Fishbein - cited on original list of chemicals from Fishbein

(4) EPA-H_2O - Organic Compounds Identified in Drinking Water in the United States, Health Effects Research Laboratory, EPA, Cincinnati, Ohio, July 1, 1976

(5) NCI - cited in tabulation of chlorides prepared for NCI-CSWG by Helmes and Porrier

C - on list of vinyl chlorides for which there is information on carcinogenicity

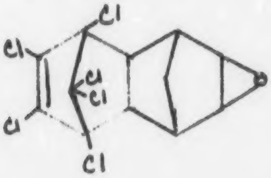
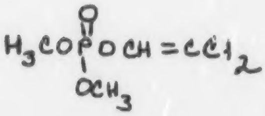
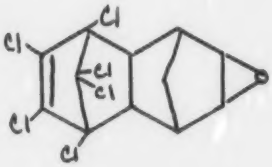
E - on list of chlorides with significant exposure

(5) Other

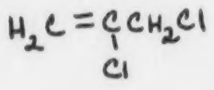
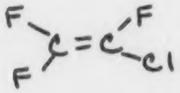
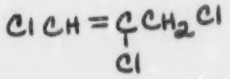
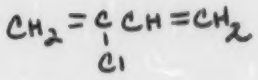
ACS
L = American Chemical Society Monograph *Chemical Carcinogenesis*, 1976 article by Lawley "Alkylating Agents"

IARC = International Agency for Research on Cancer Monograph Series, followed by Vol. No. and p.

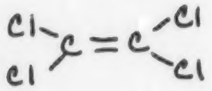
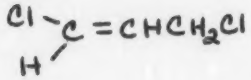
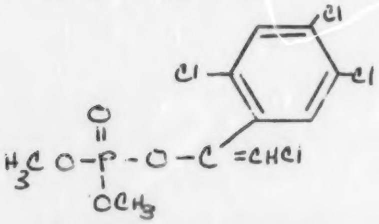
VINYL HALIDES

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI (E/C)	(6) Other
C	DIELDRIN CAS No.: 60-57-1 	C	✓		✓	✓ (E)	IARC 5, 125
A	DICHLORVOS CAS No.: 62-73-7  $H_3CO\overset{O}{\underset{OCH_3}{P}}OCH=CCl_2$	++	✓				
C	ENDRIN CAS No.: 72-20-8 	++	✓		✓	✓ (E)	IARC 5, 157
A	VINYL CHLORIDE CAS No.: 75-01-4 $H_2C=CHCl$	C	✓	✓	✓	✓ (E/C)	IARC 8, 291
A	VINYLIDENE CHLORIDE CAS No.: 75-35-4 $H_2C=CCl_2$	C?	✓	✓	✓	✓ (E/C)	

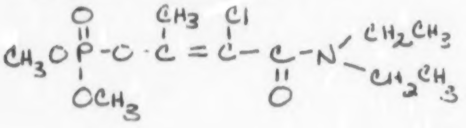
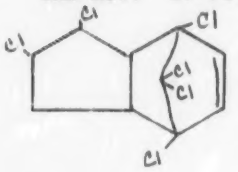
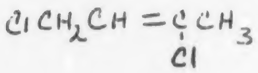
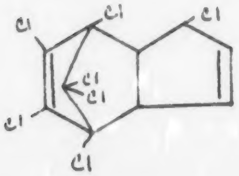
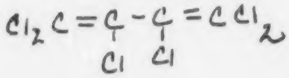
VINYL HALIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI (E/C)	(6) Other
A	2,3-DICHLOROPROPENE CAS No.: 78-88-6  $H_2C=\underset{Cl}{C}CH_2Cl$	++	✓			✓ (E)	
A	TRICHLOROETHYLENE CAS No.: 79-01-6 $ClHC=CCl_2$	C	✓	✓	✓	✓ (E/C)	IARC 11, 263
A	TRIFLUOROVINYLCHLORIDE CAS No.: 79-38-9 	++	✓			✓ (E)	
A	1,2,3-TRICHLOROPROPENE CAS No.: 96-19-5  $ClCH=\underset{Cl}{C}CH_2Cl$	++	✓			✓ (E/C)	
A	CHLOROPRENE CAS No.: 126-99-8  $CH_2=\underset{Cl}{C}CH=CH_2$	++				✓ (E)	

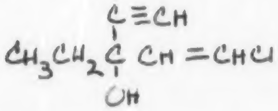
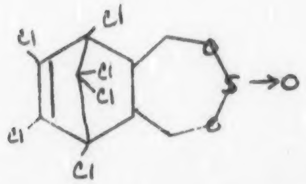
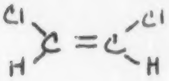
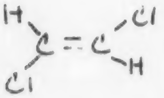
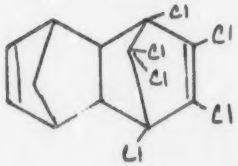
VINYL HALIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI (E/C)	(6) Other
A	PERCHLOROETHYLENE CAS No.: 127-18-4 	++	✓		✓	✓ (E)	
A	1,3-DICHLOROPROPENE CAS No.: 542-75-6 	++	✓		✓		
A	PHOSPHORIC ACID, 2-CHLORO-1-(2,4,5-TRICHLOROPHENYL)-ETHENYL DIMETHYL ESTER CAS No.: 961-11-5 	++	✓				
A	ETHYLENE, CHLOROTRIFLUORO POLYMERS CAS No.: 9002-83-9 (polymer saturated, no longer vinyl)	0	✓				
A	VINYL CHLORIDE-VINYL ACETATE COPOLYMER CAS No.: 9002-86-2 (polymer saturated, no longer vinyl)	0	✓				

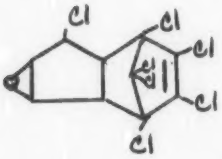
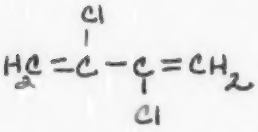
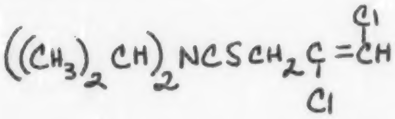
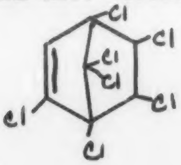
VINYL HALIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI (E/C)	(6) Other
A	PHOSPHORIC ACID, 2-CHLORO-3-(DIETHYLAMINO)-1-METHYL-3-OXO-1-PROPENYL DIMETHYL ESTER CAS No.: 13171-21-6  $CH_3O\underset{OCH_3}{\overset{O}{P}}-O-\overset{CH_3}{C}=\overset{Cl}{C}-\underset{O}{C}-N(CH_2CH_3)_2$	++	✓				
C	CHLORDANE CAS No.: 57-74-9 	++			✓	✓ (E)	
A	1,3-DICHLORO-2-BUTENE CAS No.: 76-41-0  $ClCH_2CH=\underset{Cl}{C}CH_3$	++				✓ (E)	
C	HEPTACHLOR CAS No.: 76-44-8 	++			✓	✓ (E)	
A	HEXACHLOROBUTADIENE CAS No.: 87-68-3  $Cl_2C=\underset{Cl}{C}-\underset{Cl}{C}=CCl_2$	C?			✓	✓ (C)	

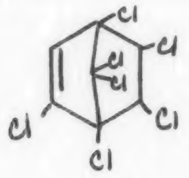
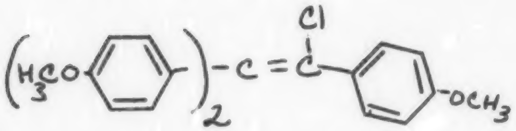
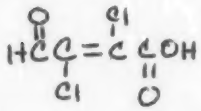
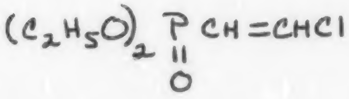
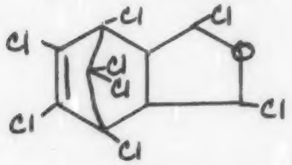
VINYL HALIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI (E/C)	(6) Other
A	ETHYCHLORVYNOL CAS No.: 113-18-8  $CH_3CH_2\underset{OH}{\overset{C\equiv CH}{C}}CH=CHCl$	++				✓ (E/C)	
C	THIODAN CAS No.: 115-29-7 	N (Innes, et al., J. Nat'l Cancer Inst., 42, 1101, 1969)				✓ (E)	
A	CIS-1,2-DICHLOROETHYLENE CAS No.: 156-59-2 	++			✓		
also mix CAS No: 25323-30-2							
	TRANS-1,2-DICHLOROETHYLENE CAS No.: 156-60-5 	++			✓		
C	ALDRIN CAS No.: 309-00-2 	++			✓	✓ (E)	

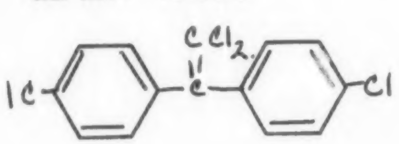
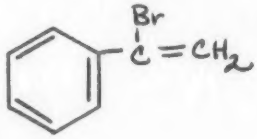
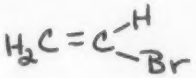
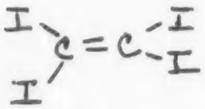
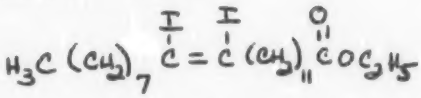
VINYL HALIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI (E/C)	(6) Other
C	HEPTACHLOR EPOXIDE CAS No.: 1024-57-3 	++			✓	✓ (E)	
A	DICHLOROBUTADIENE CAS No.: 1653-19-6  $H_2C=\overset{Cl}{C}-\underset{Cl}{C}=CH_2$	++				✓ (E)	
A	AVADEX CAS No.: 2303-16-4  $((CH_3)_2CH)_2NCSCH_2\underset{Cl}{C}=\overset{Cl}{C}H$	C				✓ (C)	
A	DICHLOROETHYNE CAS No.: 7572-29-4 $ClC\equiv CCl$	++			✓		
C	HEPTACHLORONORBORNENE, ISOMER CAS No.: 28680-45-7 	++			✓		

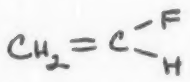
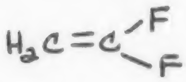
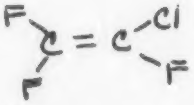
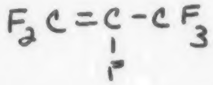
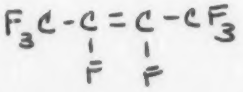
VINYL HALIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI (E/C)	(6) Other
C	**HEPTACHLORONORBORNENE** CAS No.: 55373-95-0 	++			✓		
A	**TRI-p-ANISYLCHLOROETHYLENE** CAS No.: 569-57-3 	C?	✓			✓ (C)	
A	**DICHLOROMALEALDEHYDIC ACID** CAS No.:  $\mathrm{HC(=O)C(Cl)=C(Cl)C(=O)OH}$	N? (Innes, et al., 1969)				✓ (C)	
A	**DIETHYL 2-CHLOROVINYLPHOSPHATE** CAS No.:  $(C_2H_5O)_2P(=O)CH=CHCl$	++					ACS L,170
C	**TELODRIN** CAS No.: 297-78-9 	++				✓ (C)	

VINYL HALIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H$_2$O	(5) NCI (E/C)	(6) Other
A	1,1-DICHLORO-2,2-BIS(p-CHLOROPHENYL)ETHYLENE CAS No.: 72-55-9 	C?					IARC 5, 83
A	2-BROMOSTYRENE CAS No.: 98-81-7 	++	✓				
A	ETHYLENEBROMIDE (Vinyl Bromide) CAS No.: 593-60-2 	++	✓				
A	PERIODOETHYLENE CAS No.: 513-92-8 	++	✓				
A	IODOBRASSID CAS No.: 583-87-9  $H_3C(CH_2)_7\overset{I}{C}=\overset{I}{C}(CH_2)_{11}\overset{\overset{O}{\|}}{C}OC_2H_5$	++				✓ (E)	

VINYL HALIDES (continued)

Structure Class		(1) Carcino-genicity	(2) DCP-Darr	(3) Fishbein	(4) EPA-H_2O	(5) NCI (E/C)	(6) Other
A	VINYL FLUORIDE CAS No.: 75-02-5 	+	✓				
A	1,1-DIFLUOROETHYLENE CAS No.: 75-38-7 	+	✓				
A	CHLOROTRIFLUOROETHYLENE CAS No.: 79-38-9 	++	✓				
A	HEXAFLUOROPROPENE CAS No.: 116-15-4 	+	✓				
A	PERFLUOROBUTENE-2 CAS No.: 360-89-4 	+	✓				

APPENDIX A

ADDITIONAL CHEMICALS PROVIDED BY THE PROJECT OFFICER

CHEMICALS IN ORDER BY STRUCTURAL CLASS

IA. EPOXIDES*

CAS Number	Chemical Name
60571	Dieldrin
72208	Endrin
75218	Ethylene oxide
75569	Propylene oxide
77838	α,β-Epoxy-β-methylhydrocinnamic acid, ethyl ester
81210	Dicyclopentadiene diepoxide
101906	Diglycidyl resorcinol ether
106832	n-Butyl epoxystearate
106843	Octyl epoxystearates
106887	1,2-Epoxybutane
106898	Epichlorohydrin
106901	Glycidyl acrylate
106912	Glycidyl methacrylate
106923	Allyl glycidyl ether
121391	Ethyl 3-phenyl glycidate
122601	Phenyl glycidyl ether
141377	3,4-Epoxy-6-methylcyclohexylmethyl 3,4-epoxy-6-methylcyclohexane carboxylate
285676	6-Oxabicyclo[3.1.0]hexane
286204	Cyclohexene oxide
556525	Glycidol
2426086	Butyl glycidyl ether
2751099	Oleandomycin triacetate
3083258	(2,2,2-trichloroethyl)oxirane
3132647	Epibromohydrin
3765284	2-(2-(3,3-Dimethyloxiranyl)ethenyl)-2,3-dimethyloxirane
3922905	Oleandomycin
7144652	(((1,1'-Biphenyl)-2-yloxy)methyl)oxirane
7163395	Cyclobuta(1",2":3,4;4",3":3',4')dicyclopenta(1,2-b:1',2'-b')bisoxirene, decahydro-

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*The names of the chemicals in this class were already known, so they were not included in the computer-generated lists on the following pages, as explained in Section IV.A.

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CHEMICALS IN ORDER BY STRUCTURAL CLASS (continued)

1.	1B	1000052017	SPIRONOLACTONE
2.	1B	1000077065	GIBBERELLIC ACID
3.	1C	1000057396	TRIS(2-METHYL-1-AZIRIDINYL) PHOSPHINE OXIDE
4.	1C	1009002986	POLYETHYLENIMINE
5.	1C	1002549679	2-ETHYL ETHYLENEIMINE
6.	1C	1001072522	N-2-HYDROXYETHYL ETHYLENEIMINE
7.	1C	1000545551	AZIRIDINE, 1,1',1"-PHOSPHINYLIDYNETRIS-
8.	1C	1000151564	AZIRIDINE
9.	1D	1000064675	DIETHYL SULFATE
10.	1D	1000077781	DIMETHYL SULFATE
11.	1E	1000143748	PHENOL, 4,4 -(3H-2,1-BENZOXATHIOL-3-YLIDENE) DI-, S-S-DIOXIDE
12.	1E	1001120714	1,2-OXATHIOLANE, 2,2-DIOXIDE
13.	1F	1000136287	SARCOSINE, N-[(5-CHLORO-O-TOLYL)AZO]-
14.	1F	1000120047	N-((5-CHLORO-2-METHOXYPHENYL)-AZO) SARCOSINE
15.	1F	1000103219	N-(P-TOLYLAZO) SARCOSINE
16.	1F	1000086180	N-(4-BENZAMIDO-6-METHOXY-M-TOLYL)-N-(METHYLAZO) GLYCINE
17.	1H	1000115968	2-CHLOROETHANOL, PHOSPHATE
18.	1H	1000141662	BIDRIN
19.	1H	1000512561	PHOSPHORIC ACID, TRIMETHYL ESTER
20.	1H	1000360634	PREGNA-1,4-DIENE-3,20-DIONE, 9-FLUORO-11,17-DIHYDROXY-16-METHYL-21-(PHOSPHONOOXY)-, (11.beta., 16.beta.)-
21.	1H	1000312936	PREGNA-1,4-DIENE-3,20-DIONE, 9-FLUORO-11,17-DIHYDROXY-16-METHYL-21-(PHOSPHONOOXY)-, (11.beta., 16.alpha.)-
22.	1H	1000300765	PHOSPHORIC ACID, 1,2-DIBROMO-2,2-DICHLOROETHYL DIMETHYL ESTER
23.	1H	1000298077	2-ETHYL-1-HEXANOL, HYDROGEN PHOSPHATE
24.	1H	1000131997	5 -INOSINIC ACID
25.	1H	1000130405	RIBOFLAVINE 5 -PHOSPHATE SODIUM SALT
26.	1H	1000126738	TRIBUTYL PHOSPHATE
27.	1H	1000126727	2,3-DIBROMO-1-PROPANOL, PHOSPHATE
28.	1H	1001806548	PHOSPHORIC ACID, TRIOCTYL ESTER
29.	1H	1001070037	PHOSPHORIC ACID, MONO (2-ETHYLHEXYL) ESTER
30.	1H	1000961115	PHOSPHORIC ACID, 2-CHLORO-1-(2,4,5-TRICHLOROPHENYL) ETHENYL DIMETHYL ESTER
31.	1H	1005412259	BIS(2,3-DIBROMOPROPYL) PHOSPHORI ACID
32.	1H	1005324129	MONO 2,3-DIBROMOPROPYL PHOSPHORIC ACID
33.	1H	1003991739	OCTYL PHOSPHATE
34.	1H	1007786347	00 DIMETHYL O-2-CARBOMETHOXY-1-METHYVINYL PHOSPHATE
35.	1H	1007700176	CIODRIN
36.	1H	1007558625	1,2,3-PROPANETRIOL, 1-(DIHYDROGEN PHOSPHATE), MANGANESE SALT
37.	1H	1007546283	PROPANOIC ACID, 2-(PHOSPHONOOXY)-, CALCIUM SALT
38.	1H	1007057923	DIDODECYL HYDROGEN PHOSPHATE
39.	1H	1006923224	3-HYDROXY-N-METHYL-CIS-CROTONAMIDE-DIMETHYL-PHOSPHATE
40.	1H	1024937835	5'-ADENYLIC ACID, HOMOPOLYMER
41.	1H	1019045795	OCTYL PHOSPHATE, DI POTASSIUM SALT
42.	1H	1017603428	1,2,3-PROPANETRIOL, 1-(DIHYDROGEN PHOSPHATE), SODIUM SALT
43.	1H	1013270650	5-PHOSPHORYLIBOSE 1-PYROPHOSPHATE
44.	1H	1013171216	PHOSPHORIC ACID, 2-CHLORO-3-(DIETHYLAMINO)-1-METHYL-3-OXO-1-PROPENYL DIMETHYL ESTER
45.	1H	1000078433	2,3-DICHLORO-1-PROPANOL, PHOSPHATE
46.	1H	1000078400	TRIETHYL PHOSPHATE
47.	1H	1000078513	2-BUTOXYETHANOL, PHOSPHATE
48.	1H	1000063376	5 -CYTIDYLIC ACID
49.	1H	1000058979	5 -URIDYLIC ACID
50.	1H	1000062737	PHOSPHORIC ACID, 2,2-DICHLOROVINYL DIMETHYL ESTER
51.	1I	1000075296	2-CHLOROPROPANE
52.	1I	1000075263	2-BROMOPROPANE
53.	1I	1000075003	ALKYLATING AGENTS EG ETHYL CHLORIDE
54.	1I	1000074964	BROMOETHANE
55.	1I	1000071556	METHYL CHLOROFORM
56.	1I	1000067721	HEXACHLOROETHANE
57.	1I	1000078751	1,2-DIBROMOPROPANE
58.	1I	1000076153	CHLOROPENTAFLUOROETHANE
59.	1I	1000076142	FREON 114
60.	1I	1000076120	1,1,2,2-TETRACHLORO-1,2-DIFLUOROETHANE
61.	1I	1000079345	1,1,2,2-TETRACHLOROETHANE

CHEMICALS IN ORDER BY STRUCTURAL CLASS (continued)

62.	1I	1000079276	1,1,2,2-TETRABROMOETHANE
63.	1I	1000079005	1,1,2-TRICHLOROETHANE
64.	1I	1000078875	1,2-DICHLOROPROPANE
65.	1I	1000078864	2-CHLOROBUTANE
66.	1I	1000078762	2-BROMOBUTANE
67.	1I	1000075810	1,2-DIBROMO-1,1-DICHLOROETHANE
68.	1I	1000075683	GENETRON 101
69.	1I	1005787337	BUTANE, 2-BROMO-, (R)-
70.	1I	1005787326	BUTANE, 2-BROMO-, (S)-
71.	1I	1004333566	CYCLOPROPYL BROMIDE
72.	1I	1000930289	CYCLOPENTYL CHLORIDE
73.	1I	1000662011	1,3-DICHLOROHEXAFLUOROPROPANE
74.	1I	1000661972	1,2-DICHLOROHEXAFLUOROPROPANE
75.	1I	1000626879	1,4-DIBROMOPENTANE
76.	1I	1000124732	1,2-DIBROMOTETRAFLUOROETHANE
77.	1I	1000151677	HALOTHANE
78.	1I	1000507200	PROPANE, 2-CHLORO-2-METHYL
79.	1I	1000540545	N-PROPYL CHLORIDE
80.	1I	1000111240	1,5-DIBROMOPENTANE
81.	1I	1000110532	1-BROMOPENTANE
82.	1I	1000110521	1,4-DIBROMOBUTANE
83.	1I	1000109706	1-BROMO-3-CHLOROPROPANE
84.	1I	1000109693	1-CHLOROBUTANE
85.	1I	1000109659	1-BROMOBUTANE
86.	1I	1000109648	1,3-DIBROMOPROPANE
87.	1I	1000107846	1-CHLORO-3-METHYLBUTANE
88.	1I	1000107824	1-BROMO-3-METHYLBUTANE
89.	1I	1000107813	2-BROMOPENTANE
90.	1I	1000107062	1,2-DICHLOROETHANE
91.	1I	1000106945	1-BROMOPROPANE
92.	1I	1000106934	ETHANE, 1,2-DIBROMO-
93.	1I	1000096184	1,2,3-TRICHLOROPROPANE
94.	1I	1000096128	1,2-DIBROMO-3-CHLOROPROPANE
95.	1J	1000096139	2,3-DIBROMO-1-PROPANOL
96.	1J	1000096242	3-CHLORO-1,2-PROPANEDIOL
97.	1J	1000096231	1,3-DICHLORO-2-PROPANOL
98.	1J	1000107073	2-CHLOROETHANOL
99.	1J	1000115322	4,4 -DICHLORO-A-(TRICHLOROMETHYL) BENZHYDROL
100.	1J	1000115208	2,2,2-TRICHLOROETHANOL
101.	1J	1000540512	ETHANOL, 2-BROMO-
102.	1J	1000302170	CHLORAL HYDRATE
103.	1J	1000127004	1-CHLORO-2-PROPANOL
104.	1J	1000057158	2-PROPANOL, 1,1,1-TRICHLORO-2-METHYL-
105.	1J	1000052686	(2,2,2-TRICHLORO-1-HYDROXYETHYL)-PHOSPHONIC ACID, DIMETHYL ESTER
106.	1K	1000111444	BIS(2-CHLOROETHYL) ETHER
107.	1K	1000107302	CHLOROMETHYL METHYL ETHER
108.	1K	1000110758	2-CHLOROETHYL VINYL ETHER
109.	1K	1004885023	1,1-DICHLOROMETHYL METHYL ETHER
110.	1K	1002032351	BROMOACETALDEHYDE DIETHYL ACETAL
111.	1K	1007252837	DIMETHYLBROMOACETAL
112.	1K	1000097972	CHLOROACETALDEHYDE, DIMETHYL ACETAL
113.	1K	1000076380	2,2-DICHLORO-1,1-DIFLUOROETHYL METHYL ETHER
114.	1L	1000075901	TRIFLUOROACETALDEHYDE
115.	1L	1000075876	CHLORAL
116.	1L	1000078842	ISOBUTYRALDEHYDE
117.	1L	1000079027	DICHLOROACETALDEHYDE
118.	1L	1000097961	2-ETHYLBUTYRALDEHYDE
119.	1L	1000099729	2-(P-TOLYL)-PROPIONALDEHYDE
120.	1L	1000093538	2-PHENYLPROPIONALDEHYDE
121.	1L	1000103957	CYCLAMEN ALDEHYDE
122.	1L	1000104552	CINNAMALDEHYDE

CHEMICALS IN ORDER BY STRUCTURAL CLASS (continued)

123.	1L	1000104530	3-PHENYLPROPIONALDEHYDE
124.	1L	1000104096	P-TOLYL ACETALDEHYDE
125.	1L	1021866706	ALPHA-METHYLCINNAMALDEHYDE
126.	1L	1026254922	ALPHA-ETHYLISOVALERALDEHYDE
127.	1L	1001401690	TYLOSIN
128.	1L	1001331926	AMYL CINNAMIC ALDEHYDE
129.	1L	1005392405	PERFUME (EG CITRAL)
130.	1L	1004395920	P-ISOPROPYLPHENYLACETALDEHYDE
131.	1L	1004170303	2-BUTENAL
132.	1L	1000947911	DIPHENYLACETALDEHYDE
133.	1L	1002152081	FORMALDEHYDE SODIUM BISULFITE
134.	1L	1002120709	PHENOXYACETALDEHYDE
135.	1L	1000110623	VALERALDEHYDE
136.	1L	1000107891	3-HYDROXYBUTYRALDEHYDE
137.	1L	1000110418	ALDEHYDE C-12 (MNA)
138.	1L	1000107755	HYDROXYCITRONELLAL
139.	1L	1000107200	CHLOROACETALDEHYDE
140.	1L	1000107028	ACROLEIN
141.	1L	1000106230	CITRONELLAL
142.	1L	1000111308	GLUTARALDEHYDE
143.	1L	1000112549	ALDEHYDE C-12 (LAURALDEHYDE)
144.	1L	1000112458	ALDEHYDE C-11 (UNDECYLENIC)
145.	1L	1000112447	ALDEHYDE C-11 (UNDECYL)
146.	1L	1000112312	ALDEHYDE C-10
147.	1L	1000111717	HEPTANAL
148.	1L	1000123057	2-ETHYLHEXANAL
149.	1L	1000122781	PHENYL ACETALDEHYDE
150.	1L	1000124254	ALDEHYDE C-14 (MYRISTALDEHYDE)
151.	1L	1000124196	ALDEHYDE C-9 (NONANAL)
152.	1L	1000124130	ALDEHYDE C-8 (OCTANAL)
153.	1L	1000123739	CROTONALDEHYDE
154.	1L	1000123728	BUTYRALDEHYDE
155.	1L	1000123386	PROPIONALDEHYDE
156.	1L	1000123159	2-METHYLVALERALDEHYDE
157.	1L	1000496037	HEXANAL, 2-ETHYL-3-HYDROXY-
158.	1L	1000533675	D-2 DEOXYRIBOSE
159.	1L	1000143146	9-UNDECENAL
160.	1L	1000141275	CITRAL
161.	1L	1000066842	GLUCOSAMINE HYDROCHLORIDE
162.	1L	1000066251	ALDEHYDES C2-C5 PLUS MONOCYCLIC AROMATICS HEXANAL
163.	1L	1000075070	ACETALDEHYDE (ETHANAL)
164.	1L	1000050000	FORMALIN
165.	2	1000141753	BUTYRYL CHLORIDE
166.	2	1000541413	CARBONOCHLORIDIC ACID, ETHYL ESTER
167.	2	1000501531	CHLOROFORMIC ACID, BENZYL ESTER
168.	2	1000354325	TRIFLUOROACETYL CHLORIDE
169.	2	1000122043	P-NITROBENZOYL CHLORIDE
170.	2	1000122010	P-CHLOROBENZOYL CHLORIDE
171.	2	1000121904	M-NITROBENZOYL CHLORIDE
172.	2	1000112163	LAUROYL CHLORIDE
173.	2	1000112130	DECANOYL CHLORIDE
174.	2	1000112674	PALMITOYL CHLORIDE
175.	2	1000111648	OCTANOYL CHLORIDE
176.	2	1000111502	ADIPOYL CHLORIDE
177.	2	1000112776	OLEOYL CHLORIDE
178.	2	1000112765	STEAROYL CHLORIDE
179.	2	1000108236	CHLOROFORMIC ACID, ISOPROPYL ESTER
180.	2	1000111193	SEBACOYL CHLORIDE
181.	2	1002094726	1-ADAMANTANECARBOXYLIC ACID CHLORIDE
182.	2	1002528612	HEPTANOYL CHLORIDE
183.	2	1000879185	1-NAPHTHALENECARBONYL CHLORIDE

CHEMICALS IN ORDER BY STRUCTURAL CLASS (continued)

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184.      2  1000678773 PERFLUOROGLUTARYL CHLORIDE
185.      2  1000609654 BENZOYL CHLORIDE , 2-CHLORO-
186.      2  1000598210 BROMOACETYL BROMIDE
187.      2  1004462559 3-2 ,6 -DICHLOROPHENYL-5-METHYL-4-ISOXAZOLE-CARBONYL CHLORIDE
188.      2  1003282302 PROPANOYL CHLORIDE, 2,2-DIMETHYL-
189.      2  1001885149 CARBONOCHLORIDIC ACID, PHENYL ESTER
190.      2  1025629509 3-(O-CHLOROPHENYL)-5-METHYL-4-ISOXAZOLE CARBONYLCHLORIDE
191.      2  1018956871 10H-PHENOTHIAZINE-10-CARBONYL CHLORIDE
192.      2  1013889924 N-PROPYL CHLOROTHIOFORMATE
193.      2  1007144083 CHOLEST-5-EN-3-OL (3.beta.)-, CARBONOCHLORIDATE
194.      2  1000103800 PHENYLACETYL CHLORIDE
195.      2  1000102921 CINNAMOYL CHLORIDE
196.      2  1000089758 2,4-DICHLOROBENZOYL CHLORIDE
197.      2  1000088959 PHTHALOYL CHLORIDE
198.      2  1000100209 TEREPHTHALOYL CHLORIDE
199.      2  1000100072 P-ANISOYL CHLORIDE
200.      2  1000099636 ISOPHTHALOYL CHLORIDE
201.      2  1000099332 3,5-DINITROBENZOYL CHLORIDE
202.      2  1000098884 BENZOYL CHLORIDE
203.      2  1000088108 DIETHYLCARBAMOYL CHLORIDE
204.      2  1000083012 DIPHENYLCARBAMOYL CHLORIDE
205.      2  1000079221 CHLOROFORMIC ACID, METHYL ESTER
206.      2  1000079049 CHLOROACETYL CHLORIDE
207.      2  1000079038 PROPIONYL CHLORIDE
208.      2  1000079378 OXALYL CHLORIDE
209.      2  1000079301 ISOBUTYRYL CHLORIDE
210.      2  1000075445 PHOSGENE
211.      2  1000075365 ACETYL CHLORIDE
212.      2  1000076028 TRICHLOROACETYL CHLORIDE
213.      2  1000079447 DIMETHYLCARBAMOYL CHLORIDE
214.      3  1000080433 BIS(ALPHA,ALPHA-DIMETHYLBENZYL)PEROXIDE
215.      3  1000080159 ALPHA,ALPHA-DIMETHYLBENZYL HYDROPEROXIDE
216.      3  1000080477 P-MENTH-8-YL HYDROPEROXIDE
217.      3  1000075912 TERT-BUTYL HYDROPEROXIDE
218.      3  1000078637 (1,1,4,4-TETRAMETHYLTETRAMETHYLENE)BIS(TERT-BUTYL PEROXIDE)
219.      3  1000078182 1-HYDROPEROXYCYCLOHEXYL 1-HYDROXYCYCLOHEXYL PEROXIDE
220.      3  1006731368 1,1-TERT-BUTYLPEROXY-3,3,5-TRIMETHYLCYCLOHEXONE
221.      3  1007722841 HYDROGEN PEROXIDE
222.      3  1013020069 HYDROPEROXIDE, 1-METHYLPROPYL
223.      3  1001068275 2,5-DIMETHYL-2,5-(TERT-BUTYLPEROXY) HEXYNE-3
224.      3  1005809085 1,1,3,3-TETRAMETHYLBUTYL HYDROPEROXIDE
225.      3  1003025885 2,5-DIMETHYLHEXANE-2,5-DIHYDROPEROXIDE
226.      3  1002212819 1,3-BIS-TERT-BUTYLPEROXY ISOPROPYL BENZENE
227.      3  1002407945 BIS (1-HYDROXYCYCLOHEXYL) PEROXIDE
228.      3  1002372216 CARBONOPEROXOIC ACID,  O-(1,1-DIMETHYLETHYL) O-(1-METHYLETHYL)  ESTER
229.      3  1000110054 TERT-BUTYL PEROXIDE
230.      3  1000105646 PEROXYDICARBONIC ACID, DIISOPROPYL ESTER
231.     4A  1000106956 3-BROMOPROPENE
232.     4A  1000107051 3-CHLOROPROPENE
233.     4A  1000116154 HEXAFLUOROPROPENE
234.     4A  1000593602 ETHENE, BROMO-
235.     4A  1000760236 3,4-DICHLOROBUTENE-1
236.     4A  1009002862 VINYL CHLORIDE-VINYL ACETATE COPOLYMER (EG PVC)
237.     4A  1009002839 ETHYLENE CHLOROTRIFLUORO POLYMERS
238.     4A  1000360894 PERFLUOROBUTENE-2
239.     4A  1000542756 DICHLOROPROPENE
240.     4A  1000513928 TETRAIDO ETHYLENE
241.     4A  1000563473 1-PROPENE, 3-CHLORO-2-METHYL-
242.     4A  1000127184 PERCHLOROETHYLENE
243.     4A  1000075387 1,1-DIFLUOROETHYLENE
244.     4A  1000075354 1,1-DICHLOROETHYLENE
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245.	4A	1000079383	CHLOROTRIFLUOROETHYLENE
246.	4A	1000079016	TRICHLOROETHYLENE
247.	4A	1000078886	2,3-DICHLOROPROPENE
248.	4A	1000096195	1,2,3-TRICHLOROPROPENE
249.	4A	1000075025	FLUOROETHYLENE
250.	4A	1000075014	CHLOROETHYLENE
251.	4B	1000067663	CHLOROFORM
252.	4B	1000074975	BROMOCHLOROMETHANE
253.	4B	1000074953	DIBROMOMETHANE
254.	4B	1000074873	CHLOROMETHANE
255.	4B	1000075252	TRIBROMOMETHANE
256.	4B	1000075092	METHYLENE CHLORIDE
257.	4B	1000056235	CARBON TETRACHLORIDE
258.	4B	1000075434	DICHLOROFLUOROMETHANE
259.	4B	1000075627	BROMOTRICHLOROMETHANE
260.	4B	1000075616	DIBROMODIFLUOROMETHANE
261.	4B	1000075456	FREON 22
262.	4B	1000075729	AEROSOL PROPELLANTS (E.G. FREON)
263.	4B	1000075718	DICHLORODIFLUOROMETHANE
264.	4B	1000075694	TRICHLOROFLUOROMETHANE
265.	4B	1000075638	BROMOTRIFLUOROMETHANE
266.	4B	1000558134	METHANE, TETRABROMO-
267.	4C	1000569573	CHLOROTRIANISENE
268.	4C	1000456428	M-FLUOROBENZYLCHLORIDE
269.	4C	1000352114	P-FLUOROBENZYLCHLORIDE
270.	4C	1000134838	CHLORO(P-CHLOROPHENYL)PHENYLMETHANE
271.	4C	1007398825	ALPHA,ALPHA,ALPHA ,ALPHA -TETRACHLOROPARAXYLENE
272.	4C	1000589151	BENZENE, 1-BROMO-4-(BROMOMETHYL)-
273.	4C	1000626164	META DICHLOROXYLENE
274.	4C	1000623256	PARA DICHLOROXYLENE
275.	4C	1000619238	ALPHA-CHLORO-M-NITROTOLUENE
276.	4C	1002362187	PARA-CHLOROMETHYL DIPHENYL OXIDE
277.	4C	1000104836	P,ALPHA-DICHLOROTOLUENE
278.	4C	1000104825	ALPHA-CHLORO-P-XYLENE
279.	4C	1000076835	CHLOROTRIPHENYLMETHANE
280.	4C	1000081196	ALPHA,ALPHA,2,6-TETRACHLOROTOLUENE
281.	4C	1000068360	2,2 -HEXACHLOROPARAXYLENE
282.	4C	1000090993	CHLORODIPHENYLMETHANE
283.	4C	1000086522	1-(CHLOROMETHYL)NAPHTHALENE
284.	4C	1000098873	ALPHA,ALPHA-DICHLOROTOLUENE
285.	4C	1000100118	ALPHA-BROMO-P-NITROTOLUENE
286.	4C	1000098817	ALPHA-BROMOSTYRENE
287.	4C	1000098077	ALPHA,ALPHA,ALPHA-TRICHLOROTOLUENE
288.	4C	1000100447	ALPHA-CHLOROTOLUENE
289.	4C	1000100390	ALPHA-BROMOTOLUENE
290.	4D	1000092046	2-CHLORO-4-PHENYLPHENOL
291.	4D	1002974927	POLYCHLOROBIPHENYL
292.	4D	1002051243	POLYCHLORINATED BIPHENYLS
293.	4D	1002050682	POLYCHLOROBIPHENYL
294.	4D	1002050671	POLYCHLOROBIPHENYL
295.	4E	1000081345	5,13-DIBROMO-8,16-PYRANTHRENEDIONE
296.	4E	1000081287	5,14-DICHLOROISOVIOLANTHRONE
297.	4E	1000081981	3,9-DIBROMO-7H-BENZ(DE)ANTHRACEN-7-ONE
298.	4E	1000081969	3-BROMO-7H-BENZ(DE)ANTHRACENE-7-ONE
299.	5A	1000080659	3-AMINO-2-OXAZOLIDINONE
300.	5A	1001743131	[1,2,4,5]TETRAZINO[1,2-a][1,2,4,5]TETRAZINE, OCTAHYDRO-
301.	5A	1001156190	TOLAZAMIDE
302.	5A	1000120774	N-(2,6-DIMETHYLMORPHOLINO)-2-BENZOTHIAZOLESULFENAMIDE
303.	5A	1000109842	2-HYDRAZINOETHANOL
304.	5A	1005906354	AMINO HEXAMETHYLENEIMINE
305.	5A	1000302012	HYDRAZINE

306.	5A	1000284651	17,18-DITHIA-3,4,11,12-TETRAAZATRICYCLO [12.2.1.1⁶,⁹]OCTADECANE
307.	5A	1000129204	4-BUTYL-1-(P-HYDROXYPHENYL)-2-PHENYL-3,5-PYRAZOLIDINEDIONE
308.	5A	1000083170	4-(BENZYLIDENEAMINO)ANTIPYRINE
309.	5A	1000083078	4-AMINOANTIPYRINE
310.	5A	1000057147	1,1-DIMETHYLHYDRAZINE
311.	5A	1000057965	SULFINPYRAZONE
312.	5A	1000060344	METHYL HYDRAZINE
313.	5A	1000050339	PHENYLBUTAZONE
314.	5B	1000593566	HYDROXYLAMINE, O-METHYL-, HYDROCHLORIDE
315.	5B	1010039540	HYDROXYLAMINE, SULFATE (2:1)
316.	5B	1001121308	2(1H)-PYRIDINETHIONE, 1-HYDROXY-
317.	5B	1001117971	N,O-DIMETHYLHYDROXYLAMINE
318.	5B	1005470111	HYDROXYLAMINE CHLORIDE
319.	5B	1003710847	N N-DIETHYLHYDROXYLAMINE
320.	5C	1016357598	1(2H)-QUINOLINECARBOXYLIC ACID, 2-ETHOXY-, ETHYL ESTER
321.	5C	1000518638	10H-PHENOTHIAZINE-10-CARBOXYLIC ACID, 2-[2-(DIMETHYLAMINO)ETHOXY]ETHYL ESTER, MONOHYDROCHLORIDE
322.	5C	1000120434	1-PIPERAZINECARBOXYLIC ACID, ETHYL ESTER
323.	5C	1000114807	(M-HYDROXYPHENYL) TRIMETHYL-AMMONIUM BROMIDE DIMETHYLCARBAMATE
324.	5C	1000051605	A(M-HYDROXYPHENYL)TRIMETHYL-AMMONIUM METHYL SULFATE DIMETHYLCARBAMATE
325.	5C	1000101268	3-HYDROXY-1-METHYLPYRIDINIUM BROMIDE DIMETHYLCARBAMATE
326.	6	1000086306	N-NITROSODIPHENYLAMINE
327.	6	1000101257	3,7-DINITROSO-1,3,5,7-TETRAAZABICYCLO(3.3.1)NONANE
328.	6	1000133551	N,N -DIMETHYL-N,N -DINITROSOTEREPHTHALAMIDE
329.	6	1000135206	N-NITROSO-N-PHENYLHYDROXYLAMINE AMMONIUM SALT
330.	6	1010024972	NITROUS OXIDE
331.	6	1000080115	N-METHYL-N-NITROSO-P-TOLUENE-SULFONAMIDE
332.	7A	1000081163	2-AMINO-1-NAPHTHALENESULFONIC ACID
333.	7A	1000081061	1-AMINO-2-NAPHTHALENESULFONIC ACID
334.	7A	1000082473	4-AMINO-5-HYDROXY-1,3-NAPHTHALENEDISULFONIC ACID
335.	7A	1000081801	9,10-DIHYDRO-1-(2-NAPHTHYLAMINO)-9,10-DIOXO-2-ANTHROIC ACID
336.	7A	1000081710	4,4 -(O-CHLOROBENZYLIDENE)-DI-2,5-XYLIDINE
337.	7A	1020325400	3,3 -DIMETHOXYBENZIDINE HYDROCHLORIDE
338.	7A	1000134918	4,4 -BIS(DIETHYLAMINO)BENZHYDROL
339.	7A	1000548629	GENTIAN VIOLET
340.	7A	1000531851	[1,1'-BIPHENYL]-4,4'-DIAMINE, DIHYDROCHLORIDE
341.	7A	1000314136	1,3-NAPHTHALENE DISULFONIC ACID, 6,6'-[(3,3'-DIMETHYL[1,1'-BIPHENYL]-4,4'-DIYL)BIS(AZO)]BIS[4-AMINO-5-HYDROXY]-, TETRASODIUM SALT
342.	7A	1000117613	4,4 -DIAMINO-2,2 -BIPHENYLDISULFONIC ACID
343.	7A	1000119937	3,3 -DIMETHYLBENZIDINE
344.	7A	1000119904	3,3 -DIMETHOXYBENZIDINE
345.	7A	1000612828	3,3 -DIMETHYLBENZIDINE HYDROCHLORIDE
346.	7A	1000101144	4,4 -METHYLENEBIS(2-CHLOROANILINE)
347.	7A	1000083647	8-AMINO-5-HYDROXY-1-NAPHTHALENESULFONIC ACID
348.	7A	1000083556	5-AMINO-1-NAPHTHOL
349.	7A	1000082871	4,4 -BENZYLIDENEDI-O-TOLUIDINE
350.	7A	1000082768	8-ANILINO-1-NAPHTHALENESULFONIC ACID
351.	7A	1000082757	8-AMINO-1-NAPHTHALENESULFONIC ACID
352.	7A	1000084866	4-AMINO-1-NAPHTHALENESULFONIC ACID
353.	7A	1000083830	4,4 -DIAMINO-5,5 -DIMETHYL-2,2 -BIPHENYLDISULFONIC ACID
354.	7A	1000101611	4,4 -METHYLENEBIS(N,N-DIMETHYLANILINE)
355.	7A	1000101779	4,4 -METHYLENEDIANILINE
356.	7A	1000091952	3,3 ,4,4 -BIPHENYLTETRAMINE
357.	7A	1000090948	4,4 -BIS(DIMETHYLAMINO)BENZOPHENONE
358.	7A	1000090937	4,4 -BIS(DIETHYLAMINO)BENZOPHENONE
359.	7A	1000090415	2-BIPHENYLAMINE
360.	7B	1000097563	C.I. SOLVENT YELLOW 3
361.	7B	1000102636	4-(2,4-XYLYLAZO)-O-TOLUIDINE
362.	7B	1000102238	M-((P-AMINOPHENYL)AZO)BENZENESULFONIC ACID
363.	7B	1000101757	4-(PHENYLAZO)DIPHENYLAMINE
364.	7B	1000101520	4-((P-NITROPHENYL)AZO)-O-ANISIDINE
365.	7B	1000101519	5-((P-AMINOPHENYL)AZO)SALICYLIC ACID
366.	7B	1000104234	P-((P-AMINOPHENYL)AZO)BENZENESULFONIC ACID

CHEMICALS IN ORDER BY STRUCTURAL CLASS (continued)

367.	7B	1000085836	C.I. SOLVENT RED 24
368.	7B	1000066635	7-((4-AMINO-5-METHOXY-O-TOLYL)AZO)-1,3-NAPHTHALENEDISULFONIC ACID
369.	7B	1003147146	1-NAPHTHALENESULFONIC ACID, 3-HYDROXY-4-[(2-HYDROXY-5-METHYLPHENYL)AZO]-
370.	7B	1001972287	DIETHYL AZODICARBOXYLATE
371.	7B	1002050148	PHENOL, 2,2'-AZOBIS-
372.	7B	1002313873	ETHOXAZENE HYDROCHLORIDE
373.	7B	1000117884	3-((2-ACETAMIDO-4-AMINOPHENYL)-AZO)-1,5-NAPHTHALENEDISULFONIC ACID
374.	7B	1000120683	4-((4-AMINO-M-TOLYL)AZO)-M-TOLUENESULFONIC ACID
375.	7B	1000314136	1,3-NAPHTHALENEDISULFONIC ACID, 6,6'-[(3,3'-DIMETHYL[1,1'-BIPHENYL]-4,4'-DIYL)BIS(AZO)]BIS[4-AMINO-5-HYDROXY]-, TETRASODIUM SALT
376.	7B	1000132387	6-ACETAMIDO-4-HYDROXY-3-((P-SULFAMOYLPHENYL)AZO)-2,7-NAPHTHALENE-DISULFONIC ACID
377.	7B	1000136283	M-((4-AMINO-3-METHOXYPHENYL)AZO)BENZENESULFONIC ACID
378.	7B	1000136403	2,6-DIAMINO-3-(PHENYLAZO)-PYRIDINE HYDROCHLORIDE
379.	7B	1000148856	4 ,4 -AZOBIS(4-BIPHENYLCARBOXYLIC ACID)
380.	7B	1000148390	6 -HYDROXY-5 -((2-HYDROXY-5-NITROPHENYL)AZO)-M-ACETOTOLUIDIDE
381.	7B	1000123773	AZODICARBONAMIDE
382.	7B	1000078671	2,2 -AZOBIS(2-METHYLPROPIONITRILE)
383.	7B	1000060117	C.I. SOLVENT YELLOW 2
384.	7B	1000060093	C.I. SOLVENT YELLOW 1
385.	9	1001070195	CARBONAZIDIC ACID, 1,1-DIMETHYLETHYL ESTER
386.	9	1018810587	BARIUM AZIDE
387.	9	1022750578	CESIUM AZIDE

CHEMICALS IN CAS NUMBER ORDER

1L	1000050000	FORMALIN
5A	1000050339	PHENYLBUTAZONE
5C	1000051605	A(M-HYDROXYPHENYL)TRIMETHYL-AMMONIUM METHYL SULFATE DIMETHYLCARBAMATE
1J	1000052017	SPIRONOLACTONE
1J	1000052686	(2,2,2-TRICHLORO-1-HYDROXYETHYL)-PHOSPHONIC ACID, DIMETHYL ESTER
4B	1000056235	CARBON TETRACHLORIDE
5A	1000057147	1,1-DIMETHYLHYDRAZINE
1J	1000057158	2-PROPANOL, 1,1,1-TRICHLORO-2-METHYL-
1C	1000057396	TRIS(2-METHYL-1-AZIRIDINYL)PHOSPHINE OXIDE
5A	1000057965	SULFINPYRAZONE
1H	1000058979	5 -URIDYLIC ACID
7B	1000060093	C.I. SOLVENT YELLOW 1
7B	1000060117	C.I. SOLVENT YELLOW 2
5A	1000060344	METHYL HYDRAZINE
1H	1000062737	PHOSPHORIC ACID, 2,2-DICHLOROVINYL DIMETHYL ESTER
1H	1000063376	5 -CYTIDYLIC ACID
1D	1000064675	DIETHYL SULFATE
1L	1000066251	ALDEHYDES C2-C5 PLUS MONOCYCLIC AROMATICS HEXANAL
1L	1000066842	GLUCOSAMINE HYDROCHLORIDE
4B	1000067663	CHLOROFORM
1I	1000067721	HEXACHLOROETHANE
4C	1000068360	2,2 -HEXACHLOROPARAXYLENE
1I	1000071556	METHYL CHLOROFORM
4B	1000074873	CHLOROMETHANE
4B	1000074953	DIBROMOMETHANE
1I	1000074964	BROMOETHANE
4B	1000074975	BROMOCHLOROMETHANE
1I	1000075003	ALKYLATING AGENTS EG ETHYL CHLORIDE
4A	1000075014	CHLOROETHYLENE
4A	1000075025	FLUOROETHYLENE
1L	1000075070	ACETALDEHYDE (ETHANAL)
4B	1000075092	METHYLENE CHLORIDE
4B	1000075252	TRIBROMOMETHANE
1I	1000075263	2-BROMOPROPANE
1I	1000075296	2-CHLOROPROPANE
4A	1000075354	1,1-DICHLOROETHYLENE
2	1000075365	ACETYL CHLORIDE
4A	1000075387	1,1-DIFLUOROETHYLENE
4B	1000075434	DICHLOROFLUOROMETHANE
2	1000075445	PHOSGENE
4B	1000075456	FREON 22
4B	1000075616	DIBROMODIFLUOROMETHANE
4B	1000075627	BROMOTRICHLOROMETHANE
4B	1000075638	BROMOTRIFLUOROMETHANE
1I	1000075683	GENETRON 101
4B	1000075694	TRICHLOROFLUOROMETHANE
4B	1000075718	DICHLORODIFLUOROMETHANE
4B	1000075729	AEROSOL PROPELLANTS (E.G. FREON)
1I	1000075810	1,2-DIBROMO-1,1-DICHLOROETHANE
1L	1000075876	CHLORAL
1L	1000075901	TRIFLUOROACETALDEHYDE
3	1000075912	TERT-BUTYL HYDROPEROXIDE
2	1000076028	TRICHLOROACETYL CHLORIDE
1I	1000076120	1,1,2,2-TETRACHLORO-1,2-DIFLUOROETHANE
1I	1000076142	FREON 114
1I	1000076153	CHLOROPENTAFLUOROETHANE
1K	1000076380	2,2-DICHLORO-1,1-DIFLUOROETHYL METHYL ETHER
4C	1000076835	CHLOROTRIPHENYLMETHANE
1B	1000077065	GIBBERELLIC ACID
1D	1000077781	DIMETHYL SULFATE
3	1000078182	1-HYDROPEROXYCYCLOHEXYL 1-HYDROXYCYCLOHEXYL PEROXIDE

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CHEMICALS IN CAS NUMBER ORDER (continued)

1H	1000078400	TRIETHYL PHOSPHATE
1H	1000078433	2,3-DICHLORO-1-PROPANOL, PHOSPHATE
1H	1000078513	2-BUTOXYETHANOL, PHOSPHATE
3	1000078637	(1,1,4,4-TETRAMETHYLTETRAMETHYLENE)BIS(TERT-BUTYL PEROXIDE)
7B	1000078671	2,2 -AZOBIS(2-METHYLPROPIONITRILE)
1I	1000078751	1,2-DIBROMOPROPANE
1I	1000078762	2-BROMOBUTANE
1L	1000078842	ISOBUTYRALDEHYDE
1I	1000078864	2-CHLOROBUTANE
1I	1000078875	1,2-DICHLOROPROPANE
4A	1000078886	2,3-DICHLOROPROPENE
1I	1000079005	1,1,2-TRICHLOROETHANE
4A	1000079016	TRICHLOROETHYLENE
1L	1000079027	DICHLOROACETALDEHYDE
2	1000079038	PROPIONYL CHLORIDE
2	1000079049	CHLOROACETYL CHLORIDE
2	1000079221	CHLOROFORMIC ACID, METHYL ESTER
1I	1000079276	1,1,2,2-TETRABROMOETHANE
2	1000079301	ISOBUTYRYL CHLORIDE
1I	1000079345	1,1,2,2-TETRACHLOROETHANE
2	1000079378	OXALYL CHLORIDE
4A	1000079389	CHLOROTRIFLUOROETHYLENE
2	1000079447	DIMETHYLCARBAMOYL CHLORIDE
6	1000080115	N-METHYL-N-NITROSO-P-TOLUENE-SULFONAMIDE
3	1000080159	ALPHA,ALPHA-DIMETHYLBENZYL HYDROPEROXIDE
3	1000080433	BIS(ALPHA,ALPHA-DIMETHYLBENZYL)PEROXIDE
3	1000080477	P-MENTH-8-YL HYDROPEROXIDE
5A	1000080659	3-AMINO-2-OXAZOLIDINONE
7A	1000081061	1-AMINO-2-NAPHTHALENESULFONIC ACID
7A	1000081163	2-AMINO-1-NAPHTHALENESULFONIC ACID
4C	1000081196	ALPHA,ALPHA,2,6-TETRACHLOROTOLUENE
4E	1000081287	5,14-DICHLOROISOVIOLANTHRONE
4E	1000081345	5,13-DIBROMO-8,16-PYRANTHRENEDIONE
7A	1000081710	4,4 -(O-CHLOROBENZYLIDENE)-DI-2,5-XYLIDINE
7A	1000081801	9,10-DIHYDRO-1-(2-NAPHTHYLAMINO)-9,10-DIOXO-2-ANTHROIC ACID
4E	1000081969	3-BROMO-7H-BENZ(DE)ANTHRACENE-7-ONE
4E	1000081981	3,9-DIBROMO-7H-BENZ(DE)ANTHRACEN-7-ONE
7A	1000082473	4-AMINO-5-HYDROXY-1,3-NAPHTHALENEDISULFONIC ACID
7A	1000082757	8-AMINO-1-NAPHTHALENESULFONIC ACID
7A	1000082768	8-ANILINO-1-NAPHTHALENESULFONIC ACID
7A	1000082871	4,4 -BENZYLIDENEDI-O-TOLUIDINE
2	1000083012	DIPHENYLCARBAMOYL CHLORIDE
5A	1000083078	4-AMINOANTIPYRINE
5A	1000083170	4-(BENZYLIDENEAMINO)ANTIPYRINE
7A	1000083556	5-AMINO-1-NAPHTHOL
7A	1000083647	4-AMINO-5-HYDROXY-1-NAPHTHALENESULFONIC ACID
7A	1000083830	4,4 -DIAMINO-5,5 -DIMETHYL-2,2 -BIPHENYLDISULFONIC ACID
7A	1000084866	4-AMINO-1-NAPHTHALENESULFONIC ACID
7B	1000085836	C.I. SOLVENT RED 24
1F	1000086180	N-(4-BENZAMIDO-6-METHOXY-M-TOLYL)-N-(METHYLAZO)GLYCINE
6	1000086306	N-NITROSODIPHENYLAMINE
4C	1000086522	1-(CHLOROMETHYL)NAPHTHALENE
7B	1000086635	7-((4-AMINO-5-METHOXY-O-TOLYL)AZO)-1,3-NAPHTHALENEDISULFONIC ACID
2	1000088108	DIETHYLCARBAMOYL CHLORIDE
2	1000088959	PHTHALOYL CHLORIDE
2	1000089758	2,4-DICHLOROBENZOYL CHLORIDE
7A	1000090415	2-BIPHENYLAMINE
7A	1000090937	4,4 -BIS(DIETHYLAMINO)BENZOPHENONE
7A	1000090948	4,4 -BIS(DIMETHYLAMINO)BENZOPHENONE
4C	1000090993	CHLORODIPHENYLMETHANE
7A	1000091952	3,3 ,4,4 -BIPHENYLTETRAMINE

4D	1000092046	2-CHLORO-4-PHENYLPHENOL
1L	1000093538	2-PHENYLPROPIONALDEHYDE
1I	1000096128	1,2-DIBROMO-3-CHLOROPROPANE
1J	1000096139	2,3-DIBROMO-1-PROPANOL
1I	1000096184	1,2,3-TRICHLOROPROPANE
4A	1000096195	1,2,3-TRICHLOROPROPENE
1J	1000096231	1,3-DICHLORO-2-PROPANOL
1J	1000096242	3-CHLORO-1,2-PROPANEDIOL
7B	1000097563	C.I. SOLVENT YELLOW 3
1L	1000097961	2-ETHYLBUTYRALDEHYDE
1K	1000097972	CHLOROACETALDEHYDE, DIMETHYL ACETAL
4C	1000098077	ALPHA,ALPHA,ALPHA-TRICHLOROTOLUENE
4C	1000098817	ALPHA-BROMOSTYRENE
4C	1000098873	ALPHA,ALPHA-DICHLOROTOLUENE
2	1000098884	BENZOYL CHLORIDE
2	1000099332	3,5-DINITROBENZOYL CHLORIDE
2	1000099638	ISOPHTHALOYL CHLORIDE
1L	1000099729	2-(P-TOLYL)-PROPIONALDEHYDE
2	1000100072	P-ANISOYL CHLORIDE
4C	1000100118	ALPHA-BROMO-P-NITROTOLUENE
2	1000100209	TEREPHTHALOYL CHLORIDE
4C	1000100390	ALPHA-BROMOTOLUENE
4C	1000100447	ALPHA-CHLOROTOLUENE
7A	1000101144	4,4 -METHYLENEBIS(2-CHLOROANILINE)
6	1000101257	3,7-DINITROSO-1,3,5,7-TETRAAZABICYCLO(3.3.1)NONANE
5C	1000101268	3-HYDROXY-1-METHYLPYRIDINIUM BROMIDE DIMETHYLCARBAMATE
7B	1000101519	5-((P-AMINOPHENYL)AZO)SALICYLIC ACID
7B	1000101520	4-((P-NITROPHENYL)AZO)-O-ANISIDINE
7A	1000101611	4,4 -METHYLENEBIS(N,N-DIMETHYLANILINE)
7B	1000101757	4-(PHENYLAZO)DIPHENYLAMINE
7A	1000101779	4,4 -METHYLENEDIANILINE
7B	1000102238	M-((P-AMINOPHENYL)AZO)BENZENESULFONIC ACID
7B	1000102636	4-(2,4-XYLYLAZO)-O-TOLUIDINE
2	1000102921	CINNAMOYL CHLORIDE
1F	1000103219	N-(P-TOLYLAZO)SARCOSINE
2	1000103800	PHENYLACETYL CHLORIDE
1L	1000103957	CYCLAMEN ALDEHYDE
1I	1000104096	P-TOLYL ACETALDEHYDE
7B	1000104234	P-((P-AMINOPHENYL)AZO)BENZENESULFONIC ACID
1L	1000104530	3-PHENYLPROPIONALDEHYDE
1L	1000104552	CINNAMALDEHYDE
4C	1000104825	ALPHA-CHLORO-P-XYLENE
4C	1000104836	P,ALPHA-DICHLOROTOLUENE
3	1000105646	PEROXYDICARBONIC ACID, DIISOPROPYL ESTER
1L	1000106230	CITRONELLAL
1I	1000106934	ETHANE, 1,2-DIBRomo-
1I	1000106945	1-BROMOPROPANE
4A	1000106956	3-BROMOPROPENE
1L	1000107028	ACROLEIN
4A	1000107051	3-CHLOROPROPENE
1I	1000107062	1,2-DICHLOROETHANE
1J	1000107073	2-CHLOROETHANOL
1L	1000107200	CHLOROACETALDEHYDE
1K	1000107302	CHLOROMETHYL METHYL ETHER
1L	1000107755	HYDROXYCITRONELLAL
1I	1000107813	2-BROMOPENTANE
1I	1000107824	1-BROMO-3-METHYLBUTANE
1I	1000107846	1-CHLORO-3-METHYLBUTANE
1L	1000107891	3-HYDROXYBUTYRALDEHYDE
2	1000108236	CHLOROFORMIC ACID, ISOPROPYL ESTER
1I	1000109648	1,3-DIBROMOPROPANE

CHEMICALS IN CAS NUMBER ORDER (continued)

1I	1000109659	1-BROMOBUTANE
1I	1000109693	1-CHLOROBUTANE
1I	1000109706	1-BROMO-3-CHLOROPROPANE
5A	1000109842	2-HYDRAZINOETHANOL
3	1000110054	TERT-BUTYL PEROXIDE
1L	1000110418	ALDEHYDE C-12 (MNA)
1I	1000110521	1,4-DIBROMOBUTANE
1I	1000110532	1-BROMOPENTANE
1L	1000110623	VALERALDEHYDE
1K	1000110758	2-CHLOROETHYL VINYL ETHER
2	1000111193	SEBACOYL CHLORIDE
1I	1000111240	1,5-DIBROMOPENTANE
1L	1000111308	GLUTARALDEHYDE
1K	1000111444	BIS(2-CHLOROETHYL) ETHER
2	1000111502	ADIPOYL CHLORIDE
2	1000111648	OCTANOYL CHLORIDE
1L	1000111717	HEPTANAL
2	1000112130	DECANOYL CHLORIDE
2	1000112163	LAUROYL CHLORIDE
1L	1000112312	ALDEHYDE C-10
1L	1000112447	ALDEHYDE C-11 (UNDECYL)
1L	1000112458	ALDEHYDE C-11 (UNDECYLENIC)
1L	1000112549	ALDEHYDE C-12 (LAURALDEHYDE)
2	1000112674	PALMITOYL CHLORIDE
2	1000112765	STEAROYL CHLORIDE
2	1000112776	OLEOYL CHLORIDE
5C	1000114807	(M-HYDROXYPHENYL) TRIMETHYL-AMMONIUM BROMIDE DIMETHYLCARBAMATE
1J	1000115208	2,2,2-TRICHLOROETHANOL
1J	1000115322	4,4 -DICHLORO-A-(TRICHLOROMETHYL) BENZHYDROL
1H	1000115968	2-CHLOROETHANOL, PHOSPHATE
4A	1000116154	HEXAFLUOROPROPENE
7A	1000117613	4,4 -DIAMINO-2,2 -BIPHENYLDISULFONIC ACID
7B	1000117884	3-((2-ACETAMIDO-4-AMINOPHENYL)-AZO)-1,5-NAPHTHALENEDISULFONIC ACID
7A	1000119904	3,3 -DIMETHOXYBENZIDINE
7A	1000119937	3,3 -DIMETHYLBENZIDINE
1F	1000120047	N-((5-CHLORO-2-METHOXYPHENYL)-AZO)SARCOSINE
5C	1000120438	1-PIPERAZINECARBOXYLIC ACID, ETHYL ESTER
7B	1000120683	4-((4-AMINO-M-TOLYL)AZO)-M-TOLUENESULFONIC ACID
5A	1000120774	N-(2,6-DIMETHYLMORPHOLINO)-2-BENZOTHIAZOLESULFENAMIDE
2	1000121904	M-NITROBENZOYL CHLORIDE
2	1000122010	P-CHLOROBENZOYL CHLORIDE
2	1000122043	P-NITROBENZOYL CHLORIDE
1I	1000122781	PHENYL ACETALDEHYDE
1L	1000123057	2-ETHYLHEXANAL
1L	1000123159	2-METHYLVALERALDEHYDE
1L	1000123386	PROPIONALDEHYDE
1L	1000123728	BUTYRALDEHYDE
1L	1000123739	CROTONALDEHYDE
7B	1000123773	AZODICARBONAMIDE
1L	1000124130	ALDEHYDE C-8 (OCTANAL)
1L	1000124196	ALDEHYDE C-9 (NONANAL)
1L	1000124254	ALDEHYDE C-14 (MYRISTALDEHYDE)
1I	1000124732	1,2-DIBROMOTETRAFLUOROETHANE
1H	1000126727	2,3-DIBROMO-1-PROPANOL, PHOSPHATE
1H	1000126738	TRIBUTYL PHOSPHATE
1J	1000127004	1-CHLORO-2-PROPANOL
4A	1000127184	PERCHLOROETHYLENE
5A	1000129204	4-BUTYL-1-(P-HYDROXYPHENYL)-2-PHENYL-3,5-PYRAZOLIDINEDIONE
1H	1000130405	RIBOFLAVINE 5 -PHOSPHATE SODIUM SALT
1H	1000131997	5 -INOSINIC ACID
7B	1000132387	6-ACETAMIDO-4-HYDROXY-3-((P-SULFAMOYLPHENYL)AZO)-2,7-NAPHTHALENE-DISULFONIC ACID

CHEMICALS IN CAS NUMBER ORDER (continued)

6	1000133551	N,N -DIMETHYL-N,N -DINITROSOTEREPHTHALAMIDE
4C	1000134838	CHLORO(P-CHLOROPHENYL)PHENYLMETHANE
7A	1000134918	4,4 -BIS(DIETHYLAMINO)BENZHYDROL
6	1000135206	N-NITROSO-N-PHENYLHYDROXYLAMINE AMMONIUM SALT
1F	1000136287	SARCOSINE, N-[(5-CHLORO-o-TOLYL)AZO]-
7B	1000136403	2,6-DIAMINO-3-(PHENYLAZO)-PYRIDINE HYDROCHLORIDE
7B	1000138283	P-((4-AMINO-3-METHOXYPHENYL)AZO)BENZENESULFONIC ACID
1L	1000141275	CITRAL
1H	1000141662	BIDRIN
2	1000141753	BUTYRYL CHLORIDE
1L	1000143146	9-UNDECENAL
1E	1000143748	PHENOL, 4,4 -(3H-2,1-BENZOXATHIOL-3-YLIDENE)DI-, S-S-DIOXIDE
7B	1000148390	6 -HYDROXY-5 -((2-HYDROXY-5-NITROPHENYL)AZO)-M-ACETOTOLUIDIDE
7B	1000148856	4 ,4 -AZOBIS(4-BIPHENYLCARBOXYLIC ACID)
1C	1000151564	AZIRIDINE
1I	1000151677	HALOTHANE
5A	1000284651	17,18-DITHIA-3,4,11,12-TETRAAZATRICYCLO[12.2.1.16,9]OCTADECANE
1H	1000298077	2-ETHYL-1-HEXANOL, HYDROGEN PHOSPHATE
1H	1000300765	PHOSPHORIC ACID, 1,2-DIBROMO-2,2-DICHLOROETHYL DIMETHYL ESTER
5A	1000302012	HYDRAZINE
1J	1000302170	CHLORAL HYDRATE
1H	1000312936	PREGNA-1,4-DIENE-3,20-DIONE, 9-FLUORO-11,17-DIHYDROXY-16-METHYL-21-(PHOSPHONOOXY)-, (11.beta., 16.alpha.)-
7B	1000314136	1,3-NAPHTHALENEDISULFONIC ACID, 6,6'-[(3,3'-DIMETHYL[1,1'-BIPHENYL] 4,4'-DIYL)BIS(AZO)]BIS[4-AMINO-5-HYDROXY]-, TETRASODIUM SALT
7A	1000314136	
4C	1000352114	P-FLUOROBENZYLCHLORIDE
2	1000354325	TRIFLUOROACETYL CHLORIDE
1H	1000360634	PREGNA-1,4-DIENE-3,20-DIONE, 9-FLUORO-11,17-DIHYDROXY-16-METHYL-21-(PHOSPHONOOXY)-, (11.beta., 16.beta.)-
4A	1000360894	PERFLUOROBUTENE-2
4C	1000456428	M-FLUOROBENZYLCHLORIDE
1L	1000496037	HEXANAL, 2-ETHYL-3-HYDROXY-
2	1000501531	CHLOROFORMIC ACID, BENZYL ESTER
1I	1000507200	PROPANE, 2-CHLORO-2-METHYL-
1H	1000512561	PHOSPHORIC ACID, TRIMETHYL ESTER
4A	1000513928	TETRAIODO ETHYLENE
5C	1000518638	10H-PHENOTHIAZINE-10-CARBOXYLIC ACID, 2-[2-(DIMETHYLAMINO)ETHOXY]ETHYL ESTER, MONOHYDROCHLORIDE
7A	1000531851	[1,1'-BIPHENYL]-4,4'-DIAMINE, DIHYDROCHLORIDE
1L	1000533675	D-2 DEOXYRIBOSE
1J	1000540512	ETHANOL, 2-BROMO-
1I	1000540545	N-PROPYL CHLORIDE
2	1000541413	CARBONOCHLORIDIC ACID, ETHYL ESTER
4A	1000542756	DICHLOROPROPENE
5B	1000593566	HYDROXYLAMINE, O-METHYL-, HYDROCHLORIDE
1C	1000545551	AZIRIDINE, 1,1',1''-PHOSPHINYLIDYNETRIS-
7A	1000548629	GENTIAN VIOLET
4B	1000558134	METHANE, TETRABROMO-
4A	1000563473	1-PROPENE, 3-CHLORO-2-METHYL-
4C	1000569573	CHLOROTRIANISENE
4C	1000589151	BENZENE, 1-BROMO-4-(BROMOMETHYL)-
4A	1000593602	ETHENE, BROMO-
2	1000598210	BROMOACETYL BROMIDE
2	1000609654	BENZOYL CHLORIDE, 2-CHLORO-
7A	1000612828	3,3 -DIMETHYLBENZIDINE HYDROCHLORIDE
4C	1000619238	ALPHA-CHLORO-M-NITROTOLUENE
4C	1000623256	PARA DICHLOROXYLENE
4C	1000626164	META DICHLOROXYLENE
1I	1000626879	1,4-DIBROMOPENTANE
1I	1000661972	1,2-DICHLOROHEXAFLUOROPROPANE
1I	1000662011	1,3-DICHLOROHEXAFLUOROPROPANE
2	1000678773	PERFLUOROGLUTARYL CHLORIDE
4A	1000760236	3,4-DICHLOROBUTENE-1
2	1000879185	1-NAPHTHALENECARBONYL CHLORIDE

1I	1000930289	CYCLOPENTYL CHLORIDE
1L	1000947911	DIPHENYLACETALDEHYDE
1H	1000961115	PHOSPHORIC ACID, 2-CHLORO-1-(2,4,5-TRICHLOROPHENYL)ETHENYL DIMETHYL ESTER
3	1001068275	2,5-DIMETHYL-2,5-(TERT-BUTYLPEROXY) HEXYNE-3
1H	1001070037	PHOSPHORIC ACID, MONO (2-ETHYLHEXYL) ESTER
3	1001070195	CARBONAZIDIC ACID, 1,1-DIMETHYLETHYL ESTER
1C	1001072522	N-2-HYDROXYETHYL ETHYLENEIMINE
5B	1001117971	N,O-DIMETHYLHYDROXYLAMINE
1E	1001120714	1,2-OXATHIOLANE, 2,2-DIOXIDE
5B	1001121308	2(1H)-PYRIDINE THIONE, 1-HYDROXY-
5A	1001156190	TOLAZAMIDE
1L	1001331926	AMYL CINNAMIC ALDEHYDE
1L	1001401690	TYLOSIN
5A	1001743131	[1,2,4,5]TETRAZINO[1,2-a][1,2,4,5]TETRAZINE, OCTAHYDRO-
1H	1001806548	PHOSPHORIC ACID, TRIOCTYL ESTER
2	1001885149	CARBONOCHLORIDIC ACID, PHENYL ESTER
7B	1001972287	DIETHYL AZODICARBOXYLATE
1K	1002032351	BROMOACETALDEHYDE DIETHYL ACETAL
7B	1002050148	PH NOL, 2,2'-AZOBIS-
4D	1002050671	POLYCHLOROBIPHENYL
4D	1002050682	POLYCHLOROBIPHENYL
4E	1002051243	POLYCHLORINATED BIPHENYLS
2	1002094726	1-ADAMANTANECARBOXYLIC ACID CHLORIDE
1L	1002129709	PHENOXYACETALDEHYDE
1L	1002152091	FORMALDEHYDE SODIUM BISULFITE
3	1002212819	1,3-BIS-TERT-BUTYLPEROXY ISOPROPYL BENZENE
7B	1002313873	ETHOXAZENE HYDROCHLORIDE
4C	1002362187	PARA-CHLOROMETHYL DIPHENYL OXIDE
3	1002372216	CARBONOPEROXOIC ACID, O-(1,1-DIMETHYLETHYL) O-(1-METHYLETHYL) ESTER
3	1002407945	BIS (1-HYDROXYCYCLOHEXYL) PEROXIDE
2	1002528612	HEPTANOYL CHLORIDE
1C	1002549679	2-ETHYL ETHYLENEIMINE
4D	1002974927	POLYCHLOROBIPHENYL
3	1003025885	2,5-DIMETHYLHEXANE-2,5-DIHYDROPEROXIDE
7P	1003147146	1-NAPHTHALENESULFONIC ACID, 3-HYDROXY-4-[(2-HYDROXY-5-METHYLPHENYL)AZO]-
2	1003282302	PROPANOYL CHLORIDE, 2,2-DIMETHYL
5B	1003710847	N N-DIETHYLHYDROXYLAMINE
1H	1003991739	OCTYL PHOSPHATE
1L	1004170303	2-BUTENAL
1I	1004333566	CYCLOPROPYL BROMIDE
1L	1004395920	P-ISOPROPYLPHENYLACETALDEHYDE
2	1004462559	3-2 ,6 -DICHLOROPHENYL-5-METHYL-4-ISOXAZOLE-CARBONYL CHLORIDE
1K	1004885023	1,1-DICHLOROMETHYL METHYL ETHER
1H	1005324129	MONO 2,3-DIBROMOPROPYL PHOSPHORIC ACID
1L	1005392405	PERFUME (EG CITRAL)
1H	1005412259	BIS(2,3-DIBROMOPROPYL) PHOSPHORI ACID
5B	1005470111	HYDROXYLAMINE CHLORIDE
1I	1005787326	BUTANE, 2-BROMO-, (S)-
1I	1005787337	BUTANE, 2-BROMO-, (R)-
3	1005809085	1,1,3,3-TETRAMETHYLBUTYL HYDROPEROXIDE
5A	1005906354	AMINO HEXAMETHYLENEIMINE
3	1006731368	1,1-TERT-BUTYLPEROXY-3,3,5-TRIMETHYLCYCLOHEXONE
1H	1006923224	3-HYDROXY-N-METHYL-CIS-CROTONAMIDE-DIMETHYL-PHOSPHATE
1H	1007057923	DIDODECYL HYDROGEN PHOSPHATE
2	1007144083	CHOLEST-5-EN-3-OL (3.beta.)-, CARBONOCHLORIDATE
1K	1007252837	DIMETHYLBROMOACETAL
4C	1007398825	ALPHA,ALPHA,ALPHA ,ALPHA -TETRACHLOROPARAXYLENE
1H	1007546283	PROPANOIC ACID, 2-(PHOSPHONOOXY)-, CALCIUM SALT
1H	1007558625	1,2,3-PROPANETRIOL, 1-(DIHYDROGEN PHOSPHATE), MANGANESE SALT
1H	1007700176	CIODRIN
3	1007722841	HYDROGEN PEROXIDE

CHEMICALS IN CAS NUMBER ORDER (continued)

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1H 1007786347 OO DIMETHYL O-2-CARBOMETHOXY-1-METHYLVINYL PHOSPHATE
4A 1009002839 ETHYLENE CHLOROTRIFLUORO POLYMERS
4A 1009002862 VINYL CHLORIDE-VINYL ACETATE COPOLYMER (EG PVC)
1C 1009002986 POLYETHYLENIMINE
6  1010024972 NITROUS OXIDE
5B 1010039540 HYDROXYLAMINE, SULFATE (2:1)
3  1013020069 HYDROPEROXIDE, 1-METHYLPROPYL
1H 1013171216 PHOSPHORIC ACID, 2-CHLORO-3-(DIETHYLAMINO)-1-METHYL-3-OXO-1-PROPENYL DIMETHYL ESTER
1H 1013270650 5-PHOSPHORYLRIBOSE 1-PYROPHOSPHATE
2  1013889924 N-PROPYL CHLOROTHIOFORMATE
5C 1016357598 1(2H)-QUINOLINECARBOXYLIC ACID, 2-ETHOXY-, ETHYL ESTER
1H 1017603428 1,2,3-PROPANETRIOL, 1-(DIHYDROGEN PHOSPHATE), SODIUM SALT
9  1018810587 BARIUM AZIDE
2  1018956871 10H-PHENOTHIAZINE-10-CARBONYL CHLORIDE
1H 1019045795 OCTYL PHOSPHATE, DI POTASSIUM SALT
7A 1020325400 3,3 -DIMETHOXYBENZIDINE HYDROCHLORIDE
1L 1021866706 ALPHA-METHYLCINNAMALDEHYDE
9  1022750578 CESIUM AZIDE
1H 1024937835 5'-ADENYLIC ACID, HOMOPOLYMER
2  1025629509 3-(O-CHLOROPHENYL)-5-METHYL-4-ISOXAZOLE CARBONYLCHLORIDE
1L 1026254922 ALPHA-ETHYLISOVALERALDEHYDE
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APPENDIX B

ECONOMIC DATA ON ADDITIONAL CLASSES

Class: Aromatic Hydrocarbons

CAS No.	Chemical Name	Price*, ¢/lb.	Annual Prod./Year/Source	Market Value, Million $	Dossiers
71432	Benzene	10.48	7000x10^6 lbs/1975/T75	730	I, II

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*Taken from Chemical Marketing Reporter, April 11, 1977. Spot price, Houston, Texas, district for barge quantities based on 7.35 pounds per gallon.

Class: Cyclic Ethers

CAS No.	Chemical Name	Price*, ¢/lb.	Annual Prod./Year/Source	Market Value, Million $	Dossiers
123911	1,4-Dioxane	73.5	18x10^6 lbs/1975/T75	13.2	I, II

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* Taken from Chemical Marketing Reporter, April 11, 1977, reflecting the list price prevailing for large lots, f.o.b. New York.

Class: Heterocyclic Amines

CAS No.	Chemical Name	Price*, ¢/lb.	Annual Prod./Year/Source	Market Value, Million $	Dossiers
148243	8-Hydroxyquinoline	620 (frt. allwd.)	>1000 lbs/1975/T75	--	--
91225	Quinoline	49 (frt. eqzd.)	>1000 lbs/1975/T75	--	--

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*Taken from Chemical Marketing Reporter, April 11, 1977, reflecting the list prices prevailing for large lots.

Class: Phosphoramides

CAS No.	Chemical Name	Price, ¢/lb.	Annual Prod./Year/Source	Market Value, Million $	Dossiers
680319	Hexamethylphosphoramide	--	>1000 lbs/1975/T75	--	I